



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 04:02 PM UTC

PDB ID : 6PZ8 / pdb_00006pz8
EMDB ID : EMD-20527
Title : MERS S0 trimer in complex with variable domain of antibody G2
Authors : Bowman, C.A.; Pallesen, J.; Ward, A.B.
Deposited on : 2019-07-31
Resolution : 4.19 Å(reported)
Based on initial model : 5W9I

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

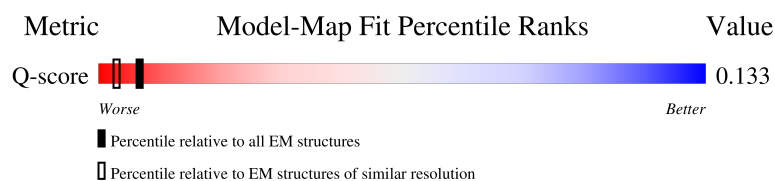
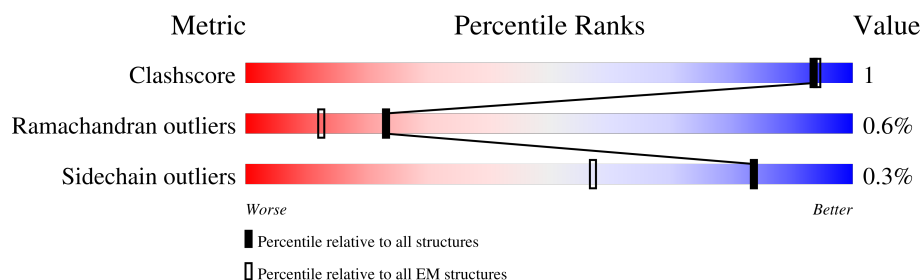
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5310 (3.70 - 4.69)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	472	7% 93% 5%
1	E	472	7% 92% 6%
1	I	472	7% 92% 6%
2	B	726	5% 64% 6% 29%

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Mol	Chain	Length	Quality of chain
2	F	726	
2	J	726	
3	C	229	
3	D	229	
3	H	229	
4	G	218	
4	K	218	
4	L	218	
5	M	2	
5	N	2	
5	O	2	
5	P	2	
5	R	2	
5	T	2	
5	U	2	
5	V	2	
5	W	2	
5	X	2	
5	Z	2	
5	b	2	
5	c	2	
5	d	2	
5	e	2	
5	f	2	
5	h	2	

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Mol	Chain	Length	Quality of chain
5	j	2	100%
6	Q	3	33% 33% 33%
6	Y	3	33% 33% 33%
6	g	3	67% 33%
7	S	5	20% 40% 60%
7	a	5	20% 40% 60%
7	i	5	20% 40% 60%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 28683 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called S protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	463	Total	C	N	O	S	0	0
			3546	2244	600	685	17		
1	E	463	Total	C	N	O	S	0	0
			3546	2244	600	685	17		
1	I	463	Total	C	N	O	S	0	0
			3546	2244	600	685	17		

- Molecule 2 is a protein called S protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	513	Total	C	N	O	S	0	0
			4010	2549	664	774	23		
2	J	513	Total	C	N	O	S	0	0
			4010	2549	664	774	23		
2	F	513	Total	C	N	O	S	0	0
			4010	2549	664	774	23		

- Molecule 3 is a protein called G2 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	116	Total	C	N	O	S	0	0
			882	559	141	178	4		
3	C	116	Total	C	N	O	S	0	0
			882	559	141	178	4		
3	D	116	Total	C	N	O	S	0	0
			882	559	141	178	4		

- Molecule 4 is a protein called G2 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	103	Total	C	N	O	S	0	0
			771	480	132	155	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	103	Total	C	N	O	S	0	0
			771	480	132	155	4		
4	K	103	Total	C	N	O	S	0	0
			771	480	132	155	4		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



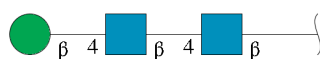
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		
5	d	2	Total	C	N	O	0	0
			28	16	2	10		
5	e	2	Total	C	N	O	0	0
			28	16	2	10		

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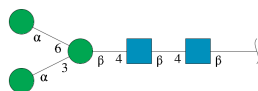
Mol	Chain	Residues	Atoms				AltConf	Trace
5	f	2	Total	C	N	O	0	0
			28	16	2	10		
5	h	2	Total	C	N	O	0	0
			28	16	2	10		
5	j	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	Q	3	Total	C	N	O	0	0
			39	22	2	15		
6	Y	3	Total	C	N	O	0	0
			39	22	2	15		
6	g	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	5	Total	C	N	O	0	0
			61	34	2	25		
7	a	5	Total	C	N	O	0	0
			61	34	2	25		
7	i	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	J	1	Total	C	N	O	0
			14	8	1	5	
8	J	1	Total	C	N	O	0
			14	8	1	5	
8	J	1	Total	C	N	O	0
			14	8	1	5	
8	J	1	Total	C	N	O	0
			14	8	1	5	
8	J	1	Total	C	N	O	0
			14	8	1	5	
8	I	1	Total	C	N	O	0
			14	8	1	5	
8	F	1	Total	C	N	O	0
			14	8	1	5	

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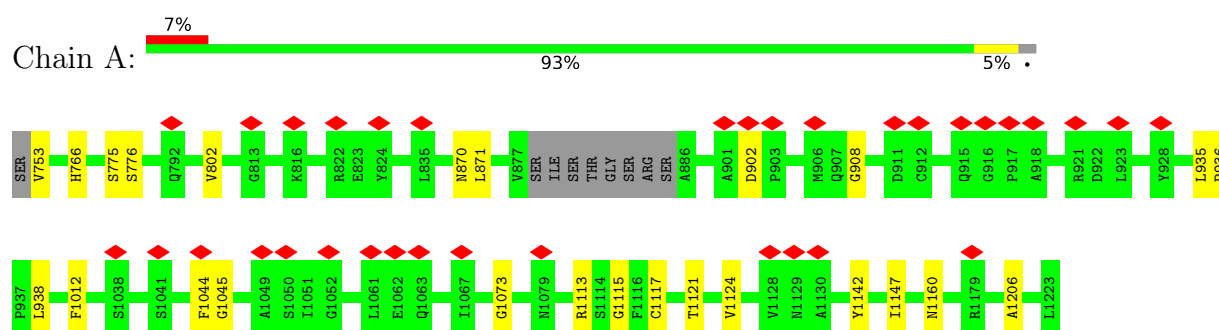
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Mol	Chain	Residues	Atoms				AltConf
8	F	1	Total	C	N	O	0
			14	8	1	5	
8	F	1	Total	C	N	O	0
			14	8	1	5	
8	F	1	Total	C	N	O	0
			14	8	1	5	
8	F	1	Total	C	N	O	0
			14	8	1	5	

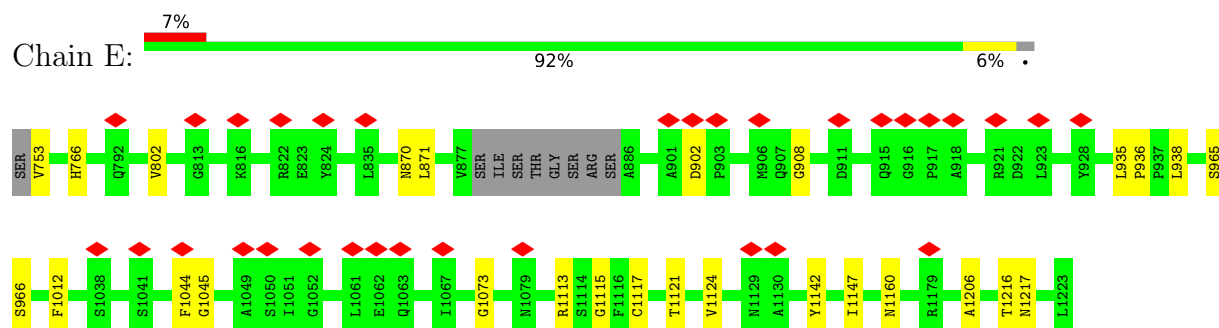
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

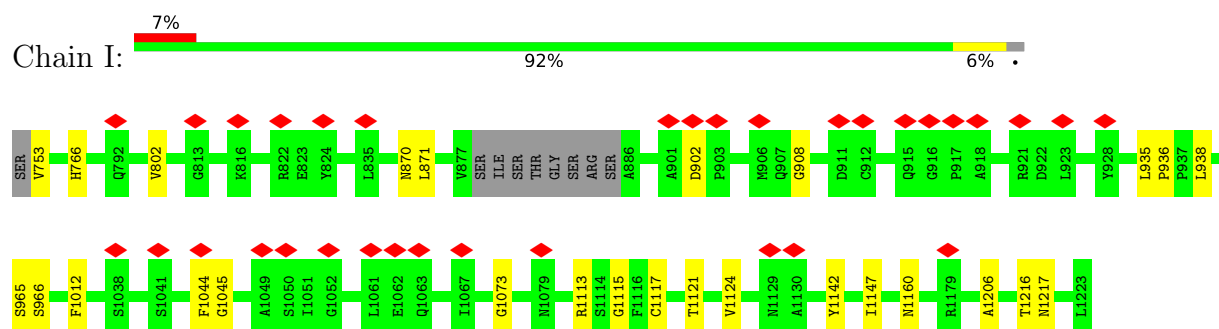
- Molecule 1: S protein



- Molecule 1: S protein

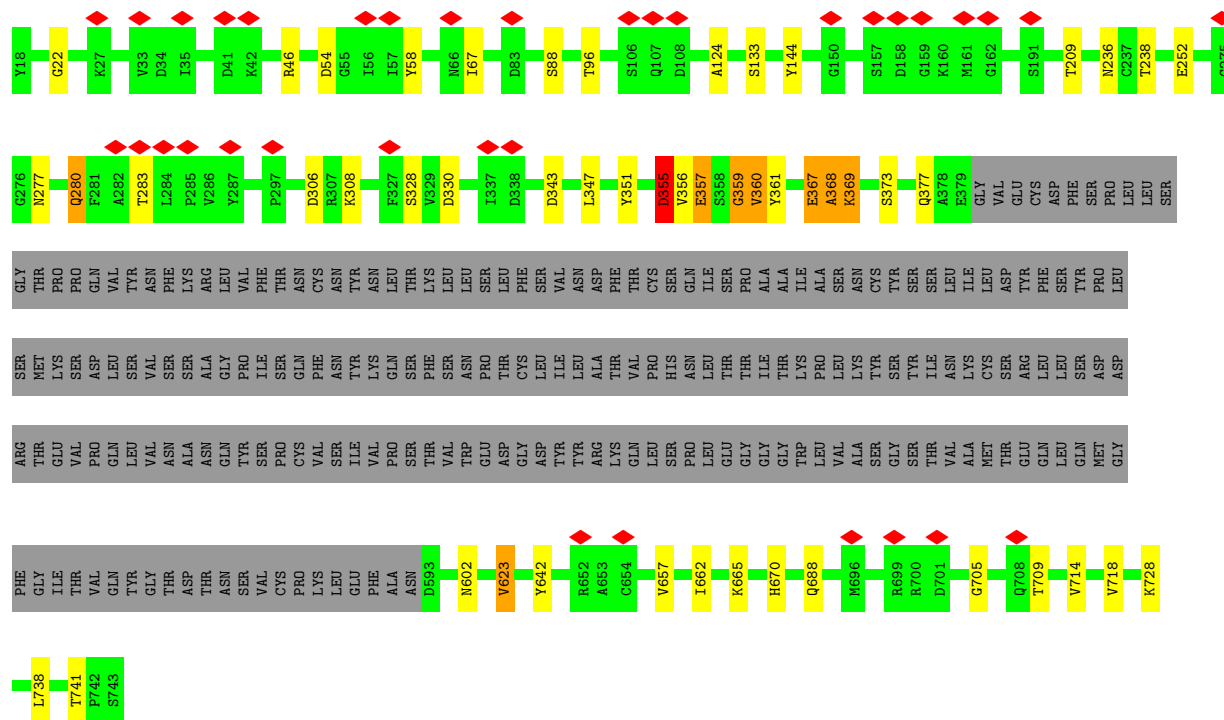


- Molecule 1: S protein

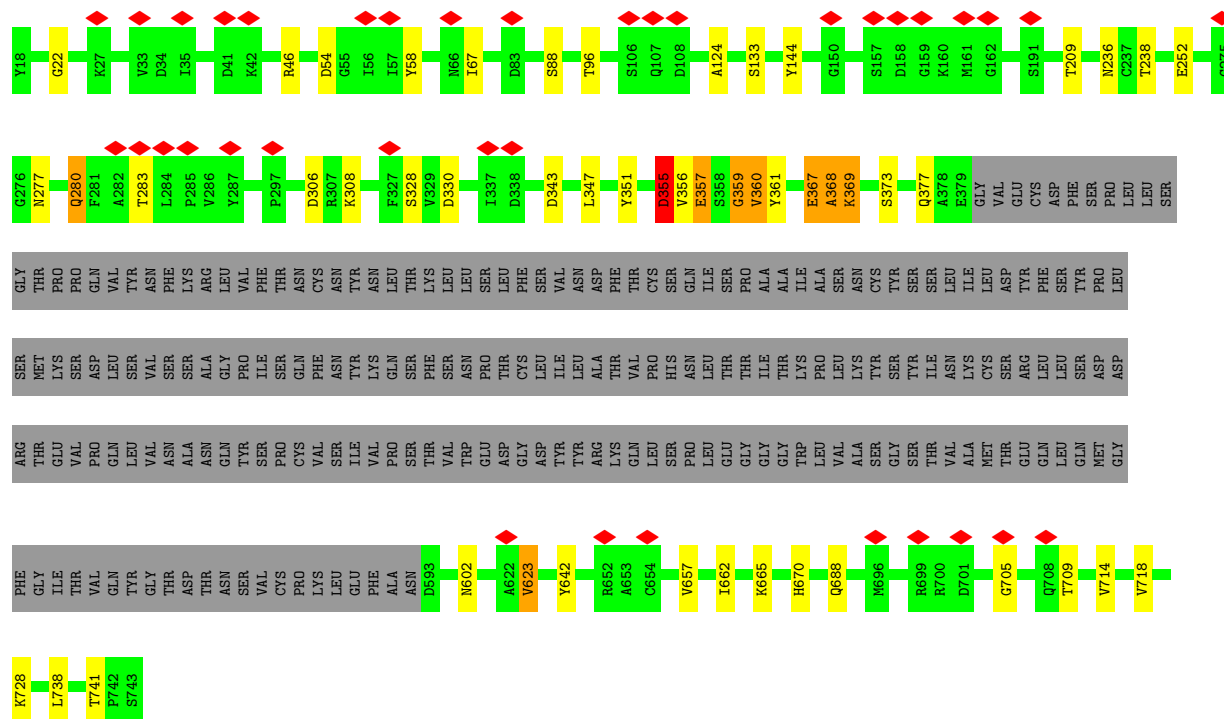


- Molecule 2: S protein



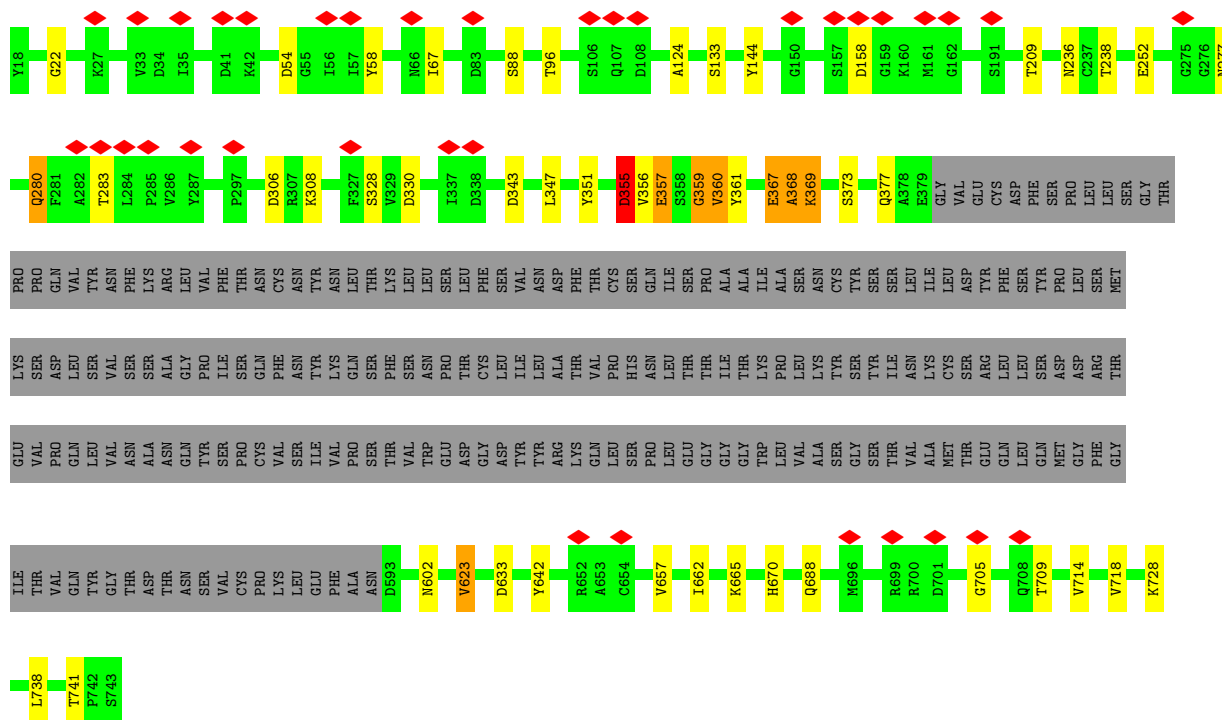


• Molecule 2: S protein

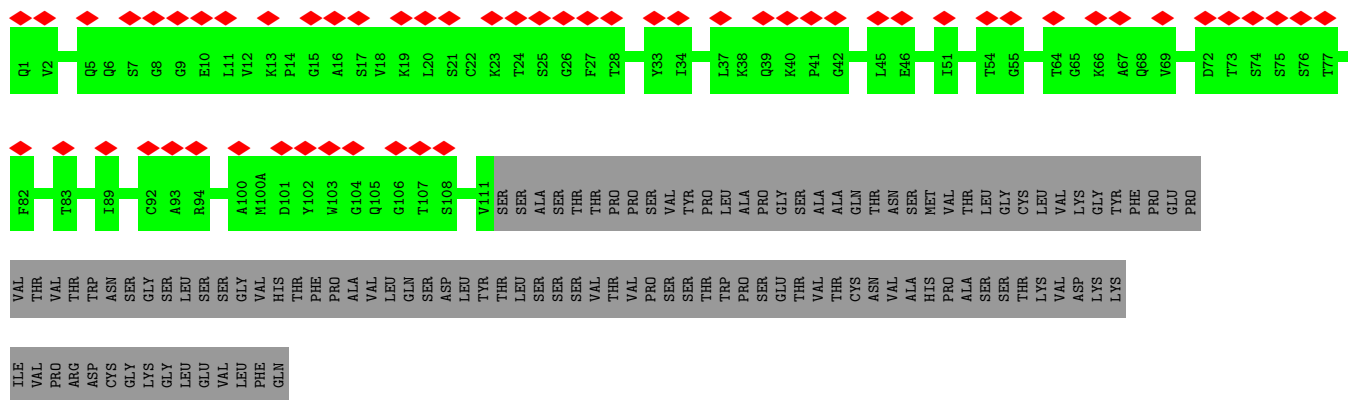


• Molecule 2: S protein

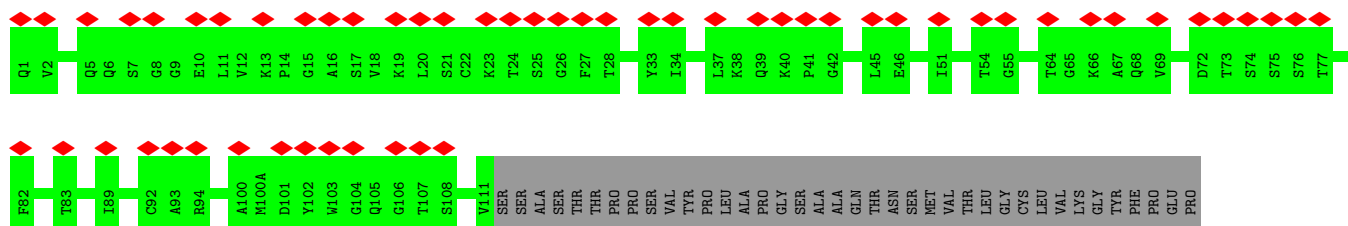




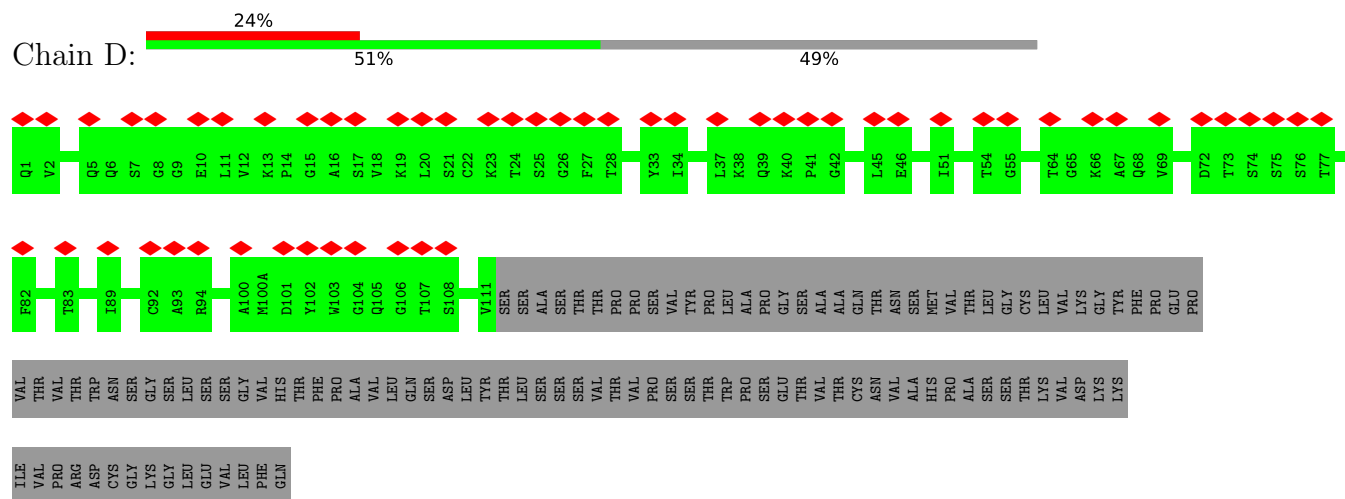
• Molecule 3: G2 heavy chain



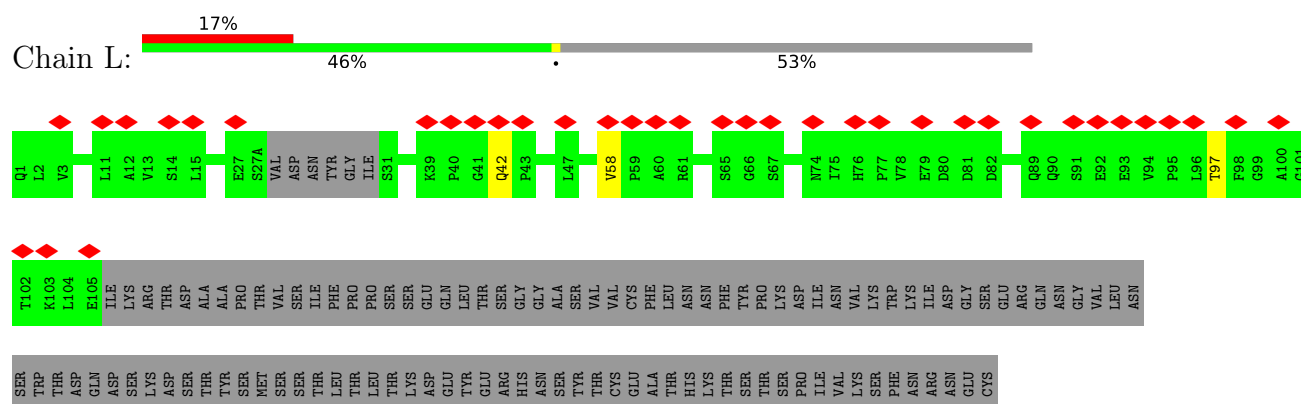
• Molecule 3: G2 heavy chain



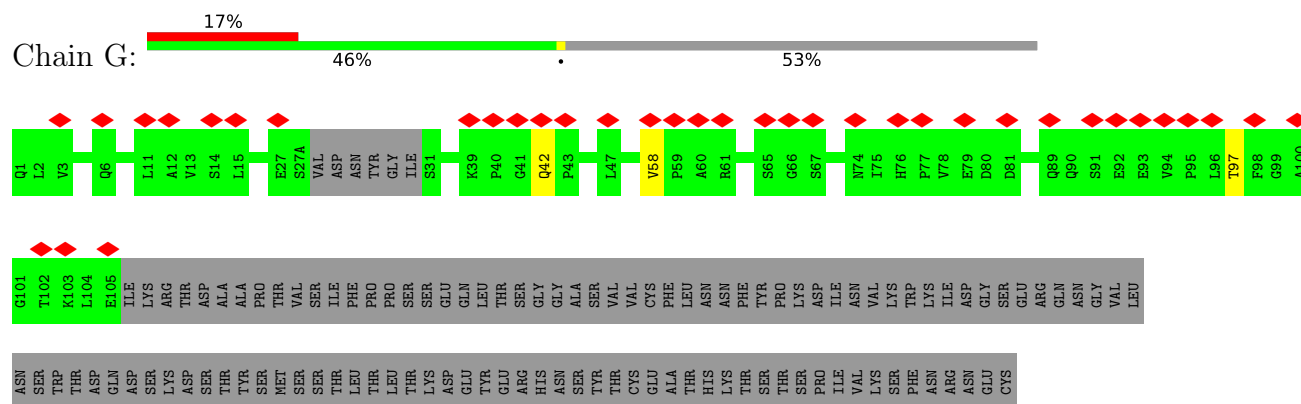
- Molecule 3: G2 heavy chain



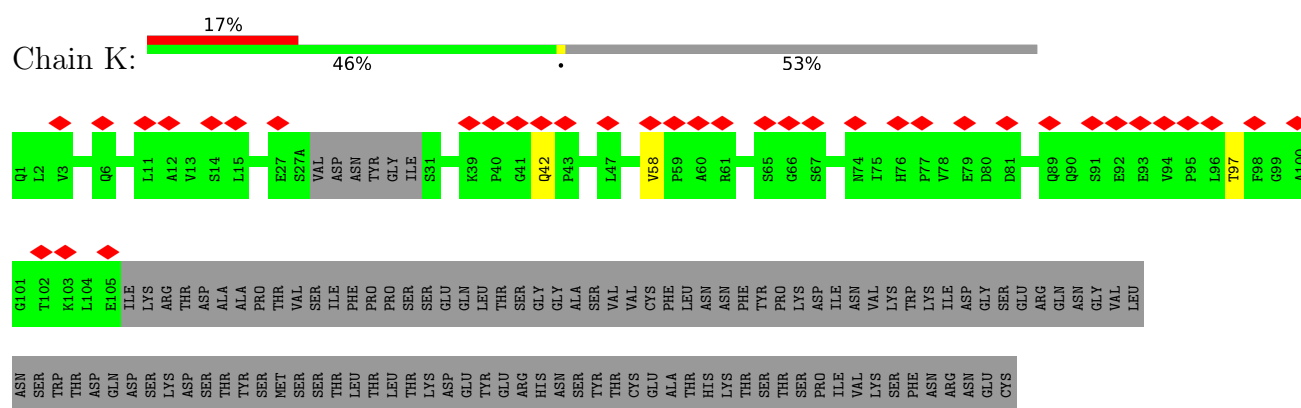
- Molecule 4: G2 light chain



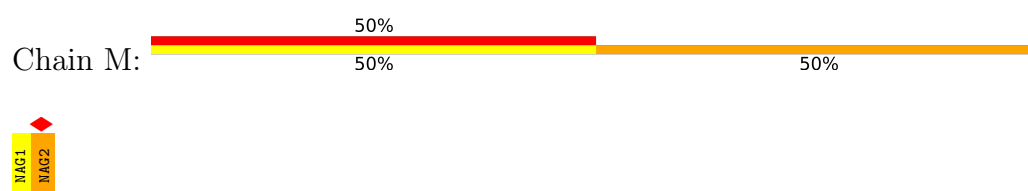
- Molecule 4: G2 light chain



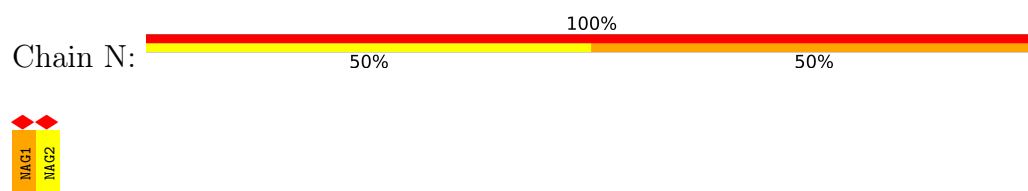
- Molecule 4: G2 light chain



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



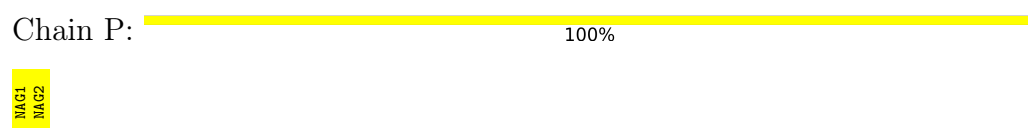
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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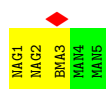
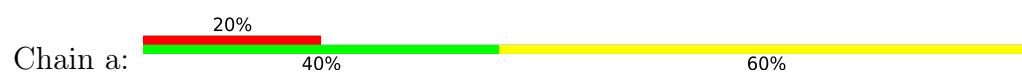


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

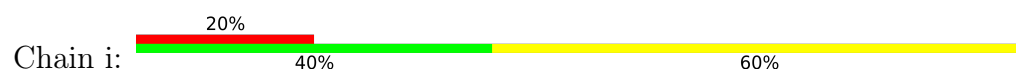


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





● Molecule 7: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	12386	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	77	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.460	Depositor
Minimum map value	-0.830	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.264	Depositor
Map size (Å)	357.0, 357.0, 357.0	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.92	0/3617	1.27	26/4918 (0.5%)
1	E	0.92	0/3617	1.27	26/4918 (0.5%)
1	I	0.92	0/3617	1.27	26/4918 (0.5%)
2	B	0.99	1/4112 (0.0%)	1.34	44/5590 (0.8%)
2	F	0.99	1/4112 (0.0%)	1.34	42/5590 (0.8%)
2	J	0.99	1/4112 (0.0%)	1.34	44/5590 (0.8%)
3	C	0.80	0/903	1.16	0/1223
3	D	0.80	0/903	1.16	0/1223
3	H	0.80	0/903	1.16	0/1223
4	G	0.85	0/787	1.23	5/1066 (0.5%)
4	K	0.85	0/787	1.23	5/1066 (0.5%)
4	L	0.85	0/787	1.23	5/1066 (0.5%)
All	All	0.93	3/28257 (0.0%)	1.29	223/38391 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	280	GLN	CG-CD	-5.40	1.38	1.52
2	J	280	GLN	CG-CD	-5.38	1.38	1.52
2	B	280	GLN	CG-CD	-5.38	1.38	1.52

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	367	GLU	N-CA-C	9.45	121.18	111.07
2	J	367	GLU	N-CA-C	9.45	121.18	111.07
2	B	367	GLU	N-CA-C	9.44	121.17	111.07
1	E	802	VAL	N-CA-C	8.47	120.98	108.45
1	A	802	VAL	N-CA-C	8.46	120.97	108.45
1	I	802	VAL	N-CA-C	8.45	120.96	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1160	ASN	CA-C-N	8.18	127.91	119.56
1	E	1160	ASN	C-N-CA	8.18	127.91	119.56
1	I	1160	ASN	CA-C-N	8.18	127.90	119.56
1	I	1160	ASN	C-N-CA	8.18	127.90	119.56
1	A	1160	ASN	CA-C-N	8.16	127.89	119.56
1	A	1160	ASN	C-N-CA	8.16	127.89	119.56
2	J	369	LYS	CA-C-N	8.05	128.07	119.78
2	J	369	LYS	C-N-CA	8.05	128.07	119.78
2	B	369	LYS	CA-C-N	8.04	128.06	119.78
2	B	369	LYS	C-N-CA	8.04	128.06	119.78
2	F	369	LYS	CA-C-N	8.01	128.03	119.78
2	F	369	LYS	C-N-CA	8.01	128.03	119.78
2	F	373	SER	N-CA-C	7.99	121.34	110.55
2	F	714	VAL	N-CA-C	7.97	120.34	108.46
2	B	373	SER	N-CA-C	7.97	121.31	110.55
2	J	373	SER	N-CA-C	7.97	121.31	110.55
2	B	714	VAL	N-CA-C	7.96	120.32	108.46
2	J	714	VAL	N-CA-C	7.96	120.31	108.46
1	E	1012	PHE	CA-CB-CG	-7.57	106.23	113.80
1	A	1012	PHE	CA-CB-CG	-7.56	106.24	113.80
1	I	1012	PHE	CA-CB-CG	-7.56	106.24	113.80
2	F	22	GLY	CA-C-N	7.44	127.39	120.03
2	F	22	GLY	C-N-CA	7.44	127.39	120.03
2	B	22	GLY	CA-C-N	7.43	127.39	120.03
2	B	22	GLY	C-N-CA	7.43	127.39	120.03
2	J	22	GLY	CA-C-N	7.42	127.38	120.03
2	J	22	GLY	C-N-CA	7.42	127.38	120.03
1	E	766	HIS	CA-C-N	7.18	127.60	119.92
1	E	766	HIS	C-N-CA	7.18	127.60	119.92
1	A	766	HIS	CA-C-N	7.17	127.59	119.92
1	A	766	HIS	C-N-CA	7.17	127.59	119.92
1	I	766	HIS	CA-C-N	7.16	127.58	119.92
1	I	766	HIS	C-N-CA	7.16	127.58	119.92
2	F	709	THR	CA-C-N	6.98	126.68	119.56
2	F	709	THR	C-N-CA	6.98	126.68	119.56
2	J	709	THR	CA-C-N	6.98	126.68	119.56
2	J	709	THR	C-N-CA	6.98	126.68	119.56
2	B	709	THR	CA-C-N	6.97	126.67	119.56
2	B	709	THR	C-N-CA	6.97	126.67	119.56
2	B	133	SER	CA-C-N	6.94	127.52	119.47
2	B	133	SER	C-N-CA	6.94	127.52	119.47
2	J	133	SER	CA-C-N	6.91	127.48	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	133	SER	C-N-CA	6.91	127.48	119.47
2	F	133	SER	CA-C-N	6.91	127.48	119.47
2	F	133	SER	C-N-CA	6.91	127.48	119.47
2	B	144	TYR	CA-C-N	6.86	126.78	119.85
2	B	144	TYR	C-N-CA	6.86	126.78	119.85
2	J	144	TYR	CA-C-N	6.86	126.78	119.85
2	J	144	TYR	C-N-CA	6.86	126.78	119.85
2	F	144	TYR	CA-C-N	6.86	126.78	119.85
2	F	144	TYR	C-N-CA	6.86	126.78	119.85
1	A	908	GLY	CA-C-N	6.85	129.76	120.38
1	A	908	GLY	C-N-CA	6.85	129.76	120.38
1	E	908	GLY	CA-C-N	6.84	129.75	120.38
1	E	908	GLY	C-N-CA	6.84	129.75	120.38
1	I	908	GLY	CA-C-N	6.82	129.72	120.38
1	I	908	GLY	C-N-CA	6.82	129.72	120.38
2	F	670	HIS	CA-CB-CG	6.72	120.52	113.80
2	J	670	HIS	CA-CB-CG	6.71	120.50	113.80
2	B	670	HIS	CA-CB-CG	6.70	120.50	113.80
2	J	705	GLY	N-CA-C	-6.70	103.86	112.10
2	F	705	GLY	N-CA-C	-6.68	103.88	112.10
2	B	705	GLY	N-CA-C	-6.66	103.91	112.10
1	E	936	PRO	CA-C-N	6.58	126.49	119.85
1	E	936	PRO	C-N-CA	6.58	126.49	119.85
1	A	936	PRO	CA-C-N	6.57	126.49	119.85
1	A	936	PRO	C-N-CA	6.57	126.49	119.85
1	I	1206	ALA	CA-C-N	6.55	126.51	119.76
1	I	1206	ALA	C-N-CA	6.55	126.51	119.76
1	A	1206	ALA	CA-C-N	6.55	126.51	119.76
1	A	1206	ALA	C-N-CA	6.55	126.51	119.76
1	E	1206	ALA	CA-C-N	6.55	126.51	119.76
1	E	1206	ALA	C-N-CA	6.55	126.51	119.76
2	B	96	THR	CA-C-N	6.54	126.51	120.03
2	B	96	THR	C-N-CA	6.54	126.51	120.03
2	J	96	THR	CA-C-N	6.54	126.50	120.03
2	J	96	THR	C-N-CA	6.54	126.50	120.03
2	F	96	THR	CA-C-N	6.50	126.46	120.03
2	F	96	THR	C-N-CA	6.50	126.46	120.03
1	I	936	PRO	CA-C-N	6.49	126.45	120.03
1	I	936	PRO	C-N-CA	6.49	126.45	120.03
4	L	58	VAL	CA-C-N	6.37	126.34	119.78
4	L	58	VAL	C-N-CA	6.37	126.34	119.78
4	G	58	VAL	CA-C-N	6.37	126.34	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	58	VAL	C-N-CA	6.37	126.34	119.78
4	K	58	VAL	CA-C-N	6.36	126.33	119.78
4	K	58	VAL	C-N-CA	6.36	126.33	119.78
1	I	902	ASP	CA-C-N	6.32	126.28	120.03
1	I	902	ASP	C-N-CA	6.32	126.28	120.03
1	E	902	ASP	CA-C-N	6.31	126.28	120.03
1	E	902	ASP	C-N-CA	6.31	126.28	120.03
1	A	902	ASP	CA-C-N	6.30	126.27	120.03
1	A	902	ASP	C-N-CA	6.30	126.27	120.03
2	F	688	GLN	CA-C-N	6.26	132.98	121.70
2	F	688	GLN	C-N-CA	6.26	132.98	121.70
2	B	67	ILE	N-CA-C	6.26	116.52	107.88
2	F	67	ILE	N-CA-C	6.26	116.52	107.88
2	B	688	GLN	CA-C-N	6.26	132.96	121.70
2	B	688	GLN	C-N-CA	6.26	132.96	121.70
2	J	688	GLN	CA-C-N	6.25	132.96	121.70
2	J	688	GLN	C-N-CA	6.25	132.96	121.70
2	J	67	ILE	N-CA-C	6.23	116.48	107.88
1	E	1117	CYS	CB-CA-C	-6.22	109.42	116.63
1	A	1117	CYS	CB-CA-C	-6.21	109.42	116.63
1	I	1117	CYS	CB-CA-C	-6.21	109.43	116.63
2	F	623	VAL	CA-C-N	-6.18	116.16	122.27
2	F	623	VAL	C-N-CA	-6.18	116.16	122.27
2	B	623	VAL	CA-C-N	-6.17	116.16	122.27
2	B	623	VAL	C-N-CA	-6.17	116.16	122.27
2	J	623	VAL	CA-C-N	-6.17	116.17	122.27
2	J	623	VAL	C-N-CA	-6.17	116.17	122.27
2	F	657	VAL	CA-C-N	6.14	126.05	119.85
2	F	657	VAL	C-N-CA	6.14	126.05	119.85
2	J	657	VAL	CA-C-N	6.12	126.03	119.85
2	J	657	VAL	C-N-CA	6.12	126.03	119.85
2	B	657	VAL	CA-C-N	6.12	126.03	119.85
2	B	657	VAL	C-N-CA	6.12	126.03	119.85
2	B	88	SER	N-CA-C	6.09	118.03	108.96
2	J	88	SER	N-CA-C	6.09	118.03	108.96
2	F	88	SER	N-CA-C	6.09	118.03	108.96
2	B	54	ASP	CA-CB-CG	6.08	118.68	112.60
2	J	54	ASP	CA-CB-CG	6.08	118.68	112.60
2	F	54	ASP	CA-CB-CG	6.06	118.66	112.60
2	B	359	GLY	N-CA-C	-6.01	107.92	115.08
2	F	359	GLY	N-CA-C	-6.01	107.93	115.08
2	F	209	THR	CA-C-N	6.00	126.44	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	209	THR	C-N-CA	6.00	126.44	119.47
2	J	359	GLY	N-CA-C	-6.00	107.94	115.08
2	B	209	THR	CA-C-N	5.99	126.42	119.47
2	B	209	THR	C-N-CA	5.99	126.42	119.47
2	J	209	THR	CA-C-N	5.98	126.41	119.47
2	J	209	THR	C-N-CA	5.98	126.41	119.47
4	G	42	GLN	CA-C-N	5.98	126.54	120.38
4	G	42	GLN	C-N-CA	5.98	126.54	120.38
1	I	1142	TYR	CA-C-N	5.98	125.89	119.85
1	I	1142	TYR	C-N-CA	5.98	125.89	119.85
1	E	1142	TYR	CA-C-N	5.97	125.89	119.85
1	E	1142	TYR	C-N-CA	5.97	125.89	119.85
4	K	42	GLN	CA-C-N	5.95	126.51	120.38
4	K	42	GLN	C-N-CA	5.95	126.51	120.38
4	L	42	GLN	CA-C-N	5.93	126.49	120.38
4	L	42	GLN	C-N-CA	5.93	126.49	120.38
1	A	1142	TYR	CA-C-N	5.93	125.83	119.85
1	A	1142	TYR	C-N-CA	5.93	125.83	119.85
1	I	1045	GLY	N-CA-C	-5.91	107.23	114.92
1	E	1045	GLY	N-CA-C	-5.91	107.23	114.92
1	A	1045	GLY	N-CA-C	-5.90	107.25	114.92
2	F	238	THR	N-CA-C	-5.89	106.23	113.41
2	J	238	THR	N-CA-C	-5.88	106.24	113.41
2	F	355	ASP	N-CA-C	-5.87	105.88	113.16
2	J	355	ASP	N-CA-C	-5.87	105.89	113.16
2	B	238	THR	N-CA-C	-5.86	106.26	113.41
2	B	355	ASP	N-CA-C	-5.86	105.90	113.16
1	E	753	VAL	CA-C-N	5.84	125.79	119.78
1	E	753	VAL	C-N-CA	5.84	125.79	119.78
1	I	753	VAL	CA-C-N	5.83	125.78	119.78
1	I	753	VAL	C-N-CA	5.83	125.78	119.78
1	A	753	VAL	CA-C-N	5.82	125.78	119.78
1	A	753	VAL	C-N-CA	5.82	125.78	119.78
1	I	1115	GLY	CA-C-N	5.68	130.82	121.39
1	I	1115	GLY	C-N-CA	5.68	130.82	121.39
1	A	1115	GLY	CA-C-N	5.67	130.81	121.39
1	A	1115	GLY	C-N-CA	5.67	130.81	121.39
1	E	1115	GLY	CA-C-N	5.66	130.79	121.39
1	E	1115	GLY	C-N-CA	5.66	130.79	121.39
1	A	1113	ARG	N-CA-C	5.65	120.23	113.23
1	I	1113	ARG	N-CA-C	5.65	120.23	113.23
1	E	1113	ARG	N-CA-C	5.63	120.21	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	97	THR	N-CA-C	5.46	117.98	109.52
4	K	97	THR	N-CA-C	5.44	117.95	109.52
4	G	97	THR	N-CA-C	5.43	117.94	109.52
2	F	623	VAL	N-CA-C	-5.34	100.14	108.95
2	B	623	VAL	N-CA-C	-5.33	100.15	108.95
2	J	728	LYS	CA-C-N	5.33	128.51	122.59
2	J	728	LYS	C-N-CA	5.33	128.51	122.59
2	F	728	LYS	CA-C-N	5.33	128.51	122.59
2	F	728	LYS	C-N-CA	5.33	128.51	122.59
2	J	623	VAL	N-CA-C	-5.33	100.16	108.95
2	F	738	LEU	CA-C-N	5.33	125.27	119.78
2	F	738	LEU	C-N-CA	5.33	125.27	119.78
2	B	728	LYS	CA-C-N	5.32	128.50	122.59
2	B	728	LYS	C-N-CA	5.32	128.50	122.59
2	J	738	LEU	CA-C-N	5.32	125.25	119.78
2	J	738	LEU	C-N-CA	5.32	125.25	119.78
2	B	738	LEU	CA-C-N	5.31	125.25	119.78
2	B	738	LEU	C-N-CA	5.31	125.25	119.78
2	F	277	ASN	CA-CB-CG	5.25	117.85	112.60
2	J	277	ASN	CA-CB-CG	5.24	117.84	112.60
2	B	277	ASN	CA-CB-CG	5.23	117.83	112.60
1	E	938	LEU	N-CA-C	5.19	118.07	111.69
1	I	938	LEU	N-CA-C	5.18	118.06	111.69
2	J	252	GLU	N-CA-C	5.17	117.87	109.24
1	A	938	LEU	N-CA-C	5.16	118.04	111.69
2	F	252	GLU	N-CA-C	5.15	117.84	109.24
2	B	252	GLU	N-CA-C	5.14	117.83	109.24
2	B	741	THR	CA-C-N	5.09	125.01	119.76
2	B	741	THR	C-N-CA	5.09	125.01	119.76
2	J	741	THR	CA-C-N	5.08	124.99	119.76
2	J	741	THR	C-N-CA	5.08	124.99	119.76
2	F	741	THR	CA-C-N	5.07	124.98	119.76
2	F	741	THR	C-N-CA	5.07	124.98	119.76
1	E	935	LEU	CA-C-N	5.06	125.59	120.38
1	E	935	LEU	C-N-CA	5.06	125.59	120.38
1	I	935	LEU	CA-C-N	5.04	125.57	120.38
1	I	935	LEU	C-N-CA	5.04	125.57	120.38
1	A	935	LEU	CA-C-N	5.03	125.56	120.38
1	A	935	LEU	C-N-CA	5.03	125.56	120.38
2	F	58	TYR	CA-C-N	5.02	124.93	119.76
2	F	58	TYR	C-N-CA	5.02	124.93	119.76
2	B	58	TYR	CA-C-N	5.02	124.93	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	58	TYR	C-N-CA	5.02	124.93	119.76
2	J	46	ARG	CA-C-N	5.02	125.00	120.03
2	J	46	ARG	C-N-CA	5.02	125.00	120.03
2	J	58	TYR	CA-C-N	5.01	124.92	119.76
2	J	58	TYR	C-N-CA	5.01	124.92	119.76
2	B	46	ARG	CA-C-N	5.01	124.99	120.03
2	B	46	ARG	C-N-CA	5.01	124.99	120.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3546	0	3474	4	0
1	E	3546	0	3474	5	0
1	I	3546	0	3474	5	0
2	B	4010	0	3811	18	0
2	F	4010	0	3811	21	0
2	J	4010	0	3811	18	0
3	C	882	0	842	0	0
3	D	882	0	842	0	0
3	H	882	0	842	0	0
4	G	771	0	740	0	0
4	K	771	0	740	0	0
4	L	771	0	740	0	0
5	M	28	0	25	1	0
5	N	28	0	25	1	0
5	O	28	0	25	1	0
5	P	28	0	25	0	0
5	R	28	0	25	0	0
5	T	28	0	25	0	0
5	U	28	0	25	0	0
5	V	28	0	25	1	0
5	W	28	0	25	0	0
5	X	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Z	28	0	25	0	0
5	b	28	0	25	0	0
5	c	28	0	25	1	0
5	d	28	0	25	1	0
5	e	28	0	25	0	0
5	f	28	0	25	0	0
5	h	28	0	25	0	0
5	j	28	0	25	0	0
6	Q	39	0	34	1	0
6	Y	39	0	34	1	0
6	g	39	0	34	2	0
7	S	61	0	52	0	0
7	a	61	0	52	0	0
7	i	61	0	52	0	0
8	A	14	0	13	0	0
8	B	70	0	65	0	0
8	E	14	0	13	0	0
8	F	70	0	65	0	0
8	I	14	0	13	0	0
8	J	70	0	65	0	0
All	All	28683	0	27543	75	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:360:VAL:HG12	2:J:360:VAL:O	1.89	0.72
2:B:360:VAL:HG12	2:B:360:VAL:O	1.89	0.72
2:F:360:VAL:HG12	2:F:360:VAL:O	1.89	0.71
2:B:360:VAL:HG22	2:B:662:ILE:HA	1.74	0.68
2:J:360:VAL:HG22	2:J:662:ILE:HA	1.74	0.68
2:F:360:VAL:HG22	2:F:662:ILE:HA	1.74	0.68
2:J:355:ASP:OD1	2:J:355:ASP:N	2.31	0.64
2:J:357:GLU:N	2:J:357:GLU:OE1	2.33	0.62
2:B:357:GLU:OE1	2:B:357:GLU:N	2.33	0.62
2:F:357:GLU:OE1	2:F:357:GLU:N	2.33	0.61
2:B:355:ASP:OD1	2:B:355:ASP:N	2.31	0.61
2:J:328:SER:OG	2:J:330:ASP:OD1	2.25	0.55
2:B:328:SER:OG	2:B:330:ASP:OD1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:328:SER:OG	2:F:330:ASP:OD1	2.25	0.54
1:I:965:SER:OG	1:I:966:SER:N	2.41	0.54
2:F:355:ASP:OD1	2:F:355:ASP:N	2.31	0.54
1:E:965:SER:OG	1:E:966:SER:N	2.41	0.53
2:B:360:VAL:O	2:B:360:VAL:CG1	2.57	0.52
2:F:360:VAL:O	2:F:360:VAL:CG1	2.57	0.52
2:B:347:LEU:HD23	2:B:361:TYR:HD1	1.74	0.52
2:F:347:LEU:HD23	2:F:361:TYR:HD1	1.74	0.52
2:B:306:ASP:OD1	2:B:308:LYS:NZ	2.44	0.51
2:J:347:LEU:HD23	2:J:361:TYR:HD1	1.74	0.51
5:O:2:NAG:O6	5:O:2:NAG:O4	2.27	0.51
2:J:306:ASP:OD1	2:J:308:LYS:NZ	2.44	0.51
2:F:343:ASP:N	2:F:343:ASP:OD1	2.43	0.51
2:F:306:ASP:OD1	2:F:308:LYS:NZ	2.44	0.50
2:J:343:ASP:N	2:J:343:ASP:OD1	2.43	0.49
2:J:360:VAL:O	2:J:360:VAL:CG1	2.57	0.49
2:B:280:GLN:NE2	2:B:283:THR:OG1	2.46	0.49
2:B:343:ASP:OD1	2:B:343:ASP:N	2.43	0.48
6:g:3:BMA:O6	6:g:3:BMA:O4	2.29	0.48
2:F:280:GLN:NE2	2:F:283:THR:OG1	2.46	0.48
5:c:2:NAG:O4	5:c:2:NAG:O6	2.27	0.48
2:J:280:GLN:NE2	2:J:283:THR:OG1	2.46	0.47
2:B:355:ASP:CB	2:B:665:LYS:HD2	2.45	0.47
2:J:355:ASP:CB	2:J:665:LYS:HD2	2.44	0.47
2:F:355:ASP:CB	2:F:665:LYS:HD2	2.45	0.47
5:M:2:NAG:O6	5:M:2:NAG:O4	2.27	0.46
2:F:124:ALA:HB3	6:g:1:NAG:H82	1.98	0.46
1:A:1147:ILE:HD12	5:N:1:NAG:H81	1.98	0.45
2:J:124:ALA:HB3	6:Y:1:NAG:H82	1.98	0.45
2:J:356:VAL:HG13	2:J:356:VAL:O	2.16	0.45
2:F:356:VAL:HG13	2:F:356:VAL:O	2.16	0.45
2:B:124:ALA:HB3	6:Q:1:NAG:H82	1.98	0.45
1:A:1044:PHE:CG	1:A:1073:GLY:HA3	2.52	0.44
1:E:1044:PHE:CG	1:E:1073:GLY:HA3	2.52	0.44
1:I:1147:ILE:HD12	5:d:1:NAG:H81	1.98	0.44
2:B:623:VAL:O	2:B:642:TYR:OH	2.31	0.44
1:E:1147:ILE:HD12	5:V:1:NAG:H81	1.98	0.44
2:J:367:GLU:O	2:J:368:ALA:HB2	2.18	0.44
1:I:1044:PHE:CG	1:I:1073:GLY:HA3	2.52	0.44
2:F:158:ASP:OD1	2:F:158:ASP:N	2.51	0.44
2:B:356:VAL:HG13	2:B:356:VAL:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:351:TYR:HB3	2:F:356:VAL:HG11	2.00	0.43
2:F:367:GLU:O	2:F:368:ALA:HB2	2.18	0.43
2:F:623:VAL:O	2:F:642:TYR:OH	2.31	0.43
2:B:367:GLU:O	2:B:368:ALA:HB2	2.18	0.43
2:F:236:ASN:OD1	2:F:236:ASN:N	2.52	0.43
1:E:1216:THR:OG1	1:E:1217:ASN:N	2.52	0.43
2:B:351:TYR:HB3	2:B:356:VAL:HG11	2.00	0.42
2:B:359:GLY:HA2	2:B:361:TYR:CE1	2.55	0.42
2:J:359:GLY:HA2	2:J:361:TYR:CE1	2.55	0.42
1:A:870:ASN:O	1:A:871:LEU:C	2.63	0.42
1:E:870:ASN:O	1:E:871:LEU:C	2.63	0.42
2:J:236:ASN:OD1	2:J:236:ASN:N	2.52	0.41
2:J:351:TYR:HB3	2:J:356:VAL:HG11	2.00	0.41
1:A:775:SER:OG	1:A:776:SER:N	2.53	0.41
1:I:1216:THR:OG1	1:I:1217:ASN:N	2.52	0.41
1:I:870:ASN:O	1:I:871:LEU:C	2.63	0.41
2:J:623:VAL:O	2:J:642:TYR:OH	2.31	0.41
2:F:359:GLY:HA2	2:F:361:TYR:CE1	2.55	0.41
2:B:236:ASN:OD1	2:B:236:ASN:N	2.52	0.41
2:F:633:ASP:OD1	2:F:633:ASP:C	2.64	0.40
2:F:360:VAL:CG2	2:F:662:ILE:HA	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/472 (97%)	442 (96%)	15 (3%)	2 (0%)	30	66
1	E	459/472 (97%)	442 (96%)	15 (3%)	2 (0%)	30	66
1	I	459/472 (97%)	442 (96%)	15 (3%)	2 (0%)	30	66
2	B	509/726 (70%)	483 (95%)	21 (4%)	5 (1%)	12	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	509/726 (70%)	483 (95%)	21 (4%)	5 (1%)	12	47
2	J	509/726 (70%)	483 (95%)	21 (4%)	5 (1%)	12	47
3	C	114/229 (50%)	113 (99%)	1 (1%)	0	100	100
3	D	114/229 (50%)	113 (99%)	1 (1%)	0	100	100
3	H	114/229 (50%)	113 (99%)	1 (1%)	0	100	100
4	G	99/218 (45%)	98 (99%)	1 (1%)	0	100	100
4	K	99/218 (45%)	98 (99%)	1 (1%)	0	100	100
4	L	99/218 (45%)	98 (99%)	1 (1%)	0	100	100
All	All	3543/4935 (72%)	3408 (96%)	114 (3%)	21 (1%)	23	58

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1124	VAL
2	B	368	ALA
2	B	602	ASN
2	B	718	VAL
1	E	1124	VAL
2	J	368	ALA
2	J	602	ASN
2	J	718	VAL
1	I	1124	VAL
2	F	368	ALA
2	F	602	ASN
2	F	718	VAL
1	A	1121	THR
1	E	1121	THR
1	I	1121	THR
2	B	377	GLN
2	J	377	GLN
2	F	377	GLN
2	B	369	LYS
2	J	369	LYS
2	F	369	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/396 (98%)	388 (100%)	0	100	100
1	E	388/396 (98%)	388 (100%)	0	100	100
1	I	388/396 (98%)	388 (100%)	0	100	100
2	B	442/635 (70%)	439 (99%)	3 (1%)	76	78
2	F	442/635 (70%)	439 (99%)	3 (1%)	76	78
2	J	442/635 (70%)	439 (99%)	3 (1%)	76	78
3	C	95/194 (49%)	95 (100%)	0	100	100
3	D	95/194 (49%)	95 (100%)	0	100	100
3	H	95/194 (49%)	95 (100%)	0	100	100
4	G	86/192 (45%)	86 (100%)	0	100	100
4	K	86/192 (45%)	86 (100%)	0	100	100
4	L	86/192 (45%)	86 (100%)	0	100	100
All	All	3033/4251 (71%)	3024 (100%)	9 (0%)	84	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	355	ASP
2	B	357	GLU
2	B	360	VAL
2	J	355	ASP
2	J	357	GLU
2	J	360	VAL
2	F	355	ASP
2	F	357	GLU
2	F	360	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	832	ASN
1	A	981	ASN
1	A	987	GLN

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Mol	Chain	Res	Type
1	A	1097	GLN
1	A	1208	GLN
2	B	98	GLN
2	B	199	ASN
2	B	280	GLN
3	H	39	GLN
4	L	38	GLN
1	E	808	GLN
1	E	812	ASN
1	E	981	ASN
1	E	987	GLN
1	E	1097	GLN
2	J	98	GLN
2	J	199	ASN
3	C	39	GLN
4	G	38	GLN
1	I	832	ASN
1	I	833	GLN
1	I	981	ASN
1	I	987	GLN
1	I	1097	GLN
1	I	1208	GLN
2	F	199	ASN
2	F	280	GLN
3	D	39	GLN
4	K	38	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

60 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	M	1	1,5	14,14,15	0.76	0	17,19,21	2.55	7 (41%)
5	NAG	M	2	5	14,14,15	0.77	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	N	1	1,5	14,14,15	0.81	1 (7%)	17,19,21	0.69	0
5	NAG	N	2	5	14,14,15	0.77	1 (7%)	17,19,21	0.80	1 (5%)
5	NAG	O	1	1,5	14,14,15	0.85	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	O	2	5	14,14,15	0.87	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	P	1	1,5	14,14,15	0.80	0	17,19,21	0.94	1 (5%)
5	NAG	P	2	5	14,14,15	0.95	1 (7%)	17,19,21	1.01	2 (11%)
6	NAG	Q	1	6,2	14,14,15	0.67	1 (7%)	17,19,21	1.12	2 (11%)
6	NAG	Q	2	6	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
6	BMA	Q	3	6	11,11,12	0.58	0	15,15,17	0.84	0
5	NAG	R	1	5,2	14,14,15	0.85	1 (7%)	17,19,21	0.90	2 (11%)
5	NAG	R	2	5	14,14,15	0.81	1 (7%)	17,19,21	0.74	1 (5%)
7	NAG	S	1	7,2	14,14,15	0.93	1 (7%)	17,19,21	1.03	1 (5%)
7	NAG	S	2	7	14,14,15	0.68	0	17,19,21	1.10	2 (11%)
7	BMA	S	3	7	11,11,12	0.71	0	15,15,17	0.78	1 (6%)
7	MAN	S	4	7	11,11,12	0.70	0	15,15,17	0.77	0
7	MAN	S	5	7	11,11,12	0.62	0	15,15,17	0.89	0
5	NAG	T	1	5,2	14,14,15	0.93	1 (7%)	17,19,21	0.73	1 (5%)
5	NAG	T	2	5	14,14,15	0.77	1 (7%)	17,19,21	0.82	1 (5%)
5	NAG	U	1	1,5	14,14,15	0.76	0	17,19,21	2.55	7 (41%)
5	NAG	U	2	5	14,14,15	0.78	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	V	1	1,5	14,14,15	0.81	1 (7%)	17,19,21	0.70	0
5	NAG	V	2	5	14,14,15	0.77	1 (7%)	17,19,21	0.80	1 (5%)
5	NAG	W	1	1,5	14,14,15	0.85	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	W	2	5	14,14,15	0.88	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	X	1	1,5	14,14,15	0.80	0	17,19,21	0.94	1 (5%)
5	NAG	X	2	5	14,14,15	0.95	1 (7%)	17,19,21	1.01	2 (11%)
6	NAG	Y	1	6,2	14,14,15	0.66	1 (7%)	17,19,21	1.12	2 (11%)
6	NAG	Y	2	6	14,14,15	0.74	0	17,19,21	1.01	1 (5%)
6	BMA	Y	3	6	11,11,12	0.58	0	15,15,17	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	Z	1	5,2	14,14,15	0.85	1 (7%)	17,19,21	0.90	2 (11%)
5	NAG	Z	2	5	14,14,15	0.82	1 (7%)	17,19,21	0.73	1 (5%)
7	NAG	a	1	7,2	14,14,15	0.94	1 (7%)	17,19,21	1.03	1 (5%)
7	NAG	a	2	7	14,14,15	0.68	1 (7%)	17,19,21	1.11	2 (11%)
7	BMA	a	3	7	11,11,12	0.71	0	15,15,17	0.78	1 (6%)
7	MAN	a	4	7	11,11,12	0.70	0	15,15,17	0.77	0
7	MAN	a	5	7	11,11,12	0.63	0	15,15,17	0.89	0
5	NAG	b	1	5,2	14,14,15	0.94	1 (7%)	17,19,21	0.74	1 (5%)
5	NAG	b	2	5	14,14,15	0.77	1 (7%)	17,19,21	0.81	1 (5%)
5	NAG	c	1	1,5	14,14,15	0.76	0	17,19,21	2.54	7 (41%)
5	NAG	c	2	5	14,14,15	0.78	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	d	1	1,5	14,14,15	0.82	1 (7%)	17,19,21	0.70	0
5	NAG	d	2	5	14,14,15	0.77	1 (7%)	17,19,21	0.80	1 (5%)
5	NAG	e	1	1,5	14,14,15	0.85	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	e	2	5	14,14,15	0.90	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	f	1	1,5	14,14,15	0.80	0	17,19,21	0.94	1 (5%)
5	NAG	f	2	5	14,14,15	0.95	1 (7%)	17,19,21	1.01	2 (11%)
6	NAG	g	1	6,2	14,14,15	0.66	1 (7%)	17,19,21	1.12	2 (11%)
6	NAG	g	2	6	14,14,15	0.74	0	17,19,21	1.01	1 (5%)
6	BMA	g	3	6	11,11,12	0.58	0	15,15,17	0.84	0
5	NAG	h	1	5,2	14,14,15	0.85	1 (7%)	17,19,21	0.90	2 (11%)
5	NAG	h	2	5	14,14,15	0.83	1 (7%)	17,19,21	0.74	1 (5%)
7	NAG	i	1	7,2	14,14,15	0.93	1 (7%)	17,19,21	1.03	1 (5%)
7	NAG	i	2	7	14,14,15	0.68	1 (7%)	17,19,21	1.11	2 (11%)
7	BMA	i	3	7	11,11,12	0.70	0	15,15,17	0.78	1 (6%)
7	MAN	i	4	7	11,11,12	0.70	0	15,15,17	0.76	0
7	MAN	i	5	7	11,11,12	0.63	0	15,15,17	0.90	0
5	NAG	j	1	5,2	14,14,15	0.93	1 (7%)	17,19,21	0.74	1 (5%)
5	NAG	j	2	5	14,14,15	0.78	1 (7%)	17,19,21	0.81	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	1	1,5	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	1/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	1/2/19/22	0/1/1/1
5	NAG	R	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	1/6/23/26	0/1/1/1
7	NAG	S	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1
7	BMA	S	3	7	-	2/2/19/22	0/1/1/1
7	MAN	S	4	7	-	0/2/19/22	0/1/1/1
7	MAN	S	5	7	-	1/2/19/22	0/1/1/1
5	NAG	T	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	1/6/23/26	0/1/1/1
5	NAG	U	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	U	2	5	-	1/6/23/26	0/1/1/1
5	NAG	V	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	V	2	5	-	1/6/23/26	0/1/1/1
5	NAG	W	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	NAG	X	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1
6	NAG	Y	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Y	3	6	-	1/2/19/22	0/1/1/1
5	NAG	Z	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	1/6/23/26	0/1/1/1
7	NAG	a	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	a	2	7	-	0/6/23/26	0/1/1/1
7	BMA	a	3	7	-	2/2/19/22	0/1/1/1
7	MAN	a	4	7	-	0/2/19/22	0/1/1/1
7	MAN	a	5	7	-	1/2/19/22	0/1/1/1
5	NAG	b	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	c	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	c	2	5	-	1/6/23/26	0/1/1/1
5	NAG	d	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	1/6/23/26	0/1/1/1
5	NAG	e	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	e	2	5	-	2/6/23/26	0/1/1/1
5	NAG	f	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	f	2	5	-	2/6/23/26	0/1/1/1
6	NAG	g	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	g	2	6	-	0/6/23/26	0/1/1/1
6	BMA	g	3	6	-	1/2/19/22	0/1/1/1
5	NAG	h	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	h	2	5	-	1/6/23/26	0/1/1/1
7	NAG	i	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	i	2	7	-	0/6/23/26	0/1/1/1
7	BMA	i	3	7	-	2/2/19/22	0/1/1/1
7	MAN	i	4	7	-	0/2/19/22	0/1/1/1
7	MAN	i	5	7	-	1/2/19/22	0/1/1/1
5	NAG	j	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	j	2	5	-	1/6/23/26	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	f	2	NAG	C1-C2	3.19	1.56	1.52
5	X	2	NAG	C1-C2	3.19	1.56	1.52
5	P	2	NAG	C1-C2	3.18	1.56	1.52
5	b	1	NAG	C1-C2	2.97	1.56	1.52
5	T	1	NAG	C1-C2	2.96	1.56	1.52
5	j	1	NAG	C1-C2	2.93	1.56	1.52
5	e	2	NAG	C1-C2	2.90	1.56	1.52
5	W	2	NAG	C1-C2	2.83	1.56	1.52
5	O	2	NAG	C1-C2	2.83	1.56	1.52
7	a	1	NAG	C1-C2	2.81	1.56	1.52
5	h	2	NAG	C1-C2	2.78	1.56	1.52
7	S	1	NAG	C1-C2	2.77	1.56	1.52
7	i	1	NAG	C1-C2	2.77	1.56	1.52
5	Z	2	NAG	C1-C2	2.75	1.56	1.52
5	R	2	NAG	C1-C2	2.71	1.56	1.52
5	O	1	NAG	C1-C2	2.64	1.55	1.52
5	e	1	NAG	C1-C2	2.62	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	1	NAG	C1-C2	2.62	1.55	1.52
5	R	1	NAG	C1-C2	2.60	1.55	1.52
5	Z	1	NAG	C1-C2	2.59	1.55	1.52
5	h	1	NAG	C1-C2	2.59	1.55	1.52
5	d	1	NAG	C1-C2	2.41	1.55	1.52
5	N	1	NAG	C1-C2	2.39	1.55	1.52
5	V	1	NAG	C1-C2	2.39	1.55	1.52
5	U	2	NAG	C1-C2	2.35	1.55	1.52
5	c	2	NAG	C1-C2	2.34	1.55	1.52
5	T	2	NAG	C1-C2	2.34	1.55	1.52
5	j	2	NAG	C1-C2	2.34	1.55	1.52
5	M	2	NAG	C1-C2	2.33	1.55	1.52
5	b	2	NAG	C1-C2	2.33	1.55	1.52
5	d	2	NAG	C1-C2	2.33	1.55	1.52
5	V	2	NAG	C1-C2	2.33	1.55	1.52
5	N	2	NAG	C1-C2	2.32	1.55	1.52
6	Q	1	NAG	C1-C2	2.04	1.55	1.52
6	Y	1	NAG	C1-C2	2.01	1.55	1.52
7	a	2	NAG	C1-C2	2.01	1.55	1.52
6	g	1	NAG	C1-C2	2.01	1.55	1.52
7	i	2	NAG	C1-C2	2.00	1.55	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	1	NAG	C8-C7-N2	5.65	125.48	116.12
5	M	1	NAG	C8-C7-N2	5.64	125.47	116.12
5	c	1	NAG	C2-N2-C7	5.64	130.46	122.90
5	c	1	NAG	C8-C7-N2	5.64	125.47	116.12
5	M	1	NAG	C2-N2-C7	5.63	130.45	122.90
5	U	1	NAG	C2-N2-C7	5.62	130.44	122.90
5	M	1	NAG	O4-C4-C3	-3.24	102.73	110.38
5	c	2	NAG	C4-C3-C2	-3.24	106.27	111.02
5	U	1	NAG	O4-C4-C3	-3.24	102.75	110.38
5	c	1	NAG	O4-C4-C3	-3.23	102.76	110.38
5	M	2	NAG	C4-C3-C2	-3.22	106.30	111.02
5	U	2	NAG	C4-C3-C2	-3.21	106.31	111.02
5	M	1	NAG	O7-C7-N2	-3.17	116.38	121.98
5	U	1	NAG	O7-C7-N2	-3.17	116.38	121.98
5	c	1	NAG	O7-C7-N2	-3.16	116.39	121.98
6	Y	2	NAG	C4-C3-C2	-3.10	106.48	111.02
6	Q	1	NAG	C3-C4-C5	-3.09	104.64	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	1	NAG	C3-C4-C5	-3.08	104.65	110.23
6	Q	2	NAG	C4-C3-C2	-3.08	106.51	111.02
6	g	2	NAG	C4-C3-C2	-3.08	106.51	111.02
6	g	1	NAG	C3-C4-C5	-3.07	104.66	110.23
7	a	2	NAG	C3-C4-C5	-2.78	105.20	110.23
7	S	2	NAG	C3-C4-C5	-2.77	105.20	110.23
7	i	2	NAG	C3-C4-C5	-2.77	105.21	110.23
5	f	1	NAG	C3-C4-C5	-2.71	105.33	110.23
5	X	1	NAG	C3-C4-C5	-2.69	105.35	110.23
5	P	1	NAG	C3-C4-C5	-2.69	105.36	110.23
5	O	1	NAG	C3-C4-C5	-2.62	105.47	110.23
5	e	1	NAG	C3-C4-C5	-2.62	105.48	110.23
5	W	1	NAG	C3-C4-C5	-2.62	105.48	110.23
5	W	2	NAG	C4-C3-C2	-2.58	107.23	111.02
5	e	2	NAG	C4-C3-C2	-2.58	107.24	111.02
5	O	2	NAG	C4-C3-C2	-2.58	107.24	111.02
5	M	1	NAG	C1-C2-N2	2.49	114.36	110.43
5	X	2	NAG	C4-C3-C2	-2.49	107.37	111.02
5	U	1	NAG	C1-C2-N2	2.49	114.35	110.43
5	P	2	NAG	C4-C3-C2	-2.49	107.38	111.02
5	c	1	NAG	C1-C2-N2	2.48	114.35	110.43
5	f	2	NAG	C4-C3-C2	-2.47	107.39	111.02
7	a	3	BMA	C2-C3-C4	-2.47	106.52	110.86
7	i	3	BMA	C2-C3-C4	-2.47	106.52	110.86
7	S	3	BMA	C2-C3-C4	-2.47	106.52	110.86
5	T	2	NAG	C4-C3-C2	-2.33	107.60	111.02
5	j	2	NAG	C4-C3-C2	-2.32	107.62	111.02
5	b	2	NAG	C4-C3-C2	-2.31	107.63	111.02
5	M	1	NAG	C4-C3-C2	-2.27	107.69	111.02
5	U	1	NAG	C4-C3-C2	-2.26	107.70	111.02
5	c	1	NAG	C4-C3-C2	-2.26	107.71	111.02
5	X	2	NAG	O5-C1-C2	-2.23	107.84	111.29
5	P	2	NAG	O5-C1-C2	-2.23	107.84	111.29
5	f	2	NAG	O5-C1-C2	-2.22	107.86	111.29
5	N	2	NAG	C4-C3-C2	-2.21	107.77	111.02
5	V	2	NAG	C4-C3-C2	-2.21	107.77	111.02
6	Y	1	NAG	C1-C2-N2	-2.21	106.95	110.43
6	Q	1	NAG	C1-C2-N2	-2.21	106.96	110.43
5	U	1	NAG	O7-C7-C8	-2.21	118.13	122.05
5	d	2	NAG	C4-C3-C2	-2.20	107.79	111.02
5	c	1	NAG	O7-C7-C8	-2.20	118.13	122.05
5	M	1	NAG	O7-C7-C8	-2.20	118.14	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	g	1	NAG	C1-C2-N2	-2.20	106.97	110.43
5	R	2	NAG	C4-C3-C2	-2.17	107.84	111.02
5	Z	2	NAG	C4-C3-C2	-2.15	107.86	111.02
5	h	2	NAG	C4-C3-C2	-2.15	107.87	111.02
5	h	1	NAG	C3-C4-C5	-2.09	106.44	110.23
5	Z	1	NAG	O4-C4-C3	-2.08	105.46	110.38
7	a	2	NAG	O4-C4-C3	-2.08	105.46	110.38
5	R	1	NAG	C3-C4-C5	-2.08	106.45	110.23
5	h	1	NAG	O4-C4-C3	-2.08	105.47	110.38
5	Z	1	NAG	C3-C4-C5	-2.08	106.46	110.23
5	R	1	NAG	O4-C4-C3	-2.08	105.47	110.38
7	i	2	NAG	O4-C4-C3	-2.08	105.48	110.38
7	a	1	NAG	C3-C4-C5	-2.08	106.47	110.23
7	i	1	NAG	C3-C4-C5	-2.07	106.47	110.23
7	S	1	NAG	C3-C4-C5	-2.07	106.48	110.23
7	S	2	NAG	O4-C4-C3	-2.07	105.49	110.38
5	b	1	NAG	C3-C4-C5	-2.07	106.49	110.23
5	T	1	NAG	C3-C4-C5	-2.06	106.50	110.23
5	j	1	NAG	C3-C4-C5	-2.06	106.50	110.23

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1	NAG	C1-C2-N2-C7
5	U	1	NAG	C1-C2-N2-C7
5	c	1	NAG	C1-C2-N2-C7
7	S	3	BMA	O5-C5-C6-O6
7	a	3	BMA	O5-C5-C6-O6
7	i	3	BMA	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
5	f	2	NAG	C4-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
5	Z	1	NAG	O5-C5-C6-O6
5	h	1	NAG	O5-C5-C6-O6
7	S	3	BMA	C4-C5-C6-O6
7	a	3	BMA	C4-C5-C6-O6
7	i	3	BMA	C4-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	R	1	NAG	C4-C5-C6-O6
5	Z	1	NAG	C4-C5-C6-O6
5	h	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C8-C7-N2-C2
5	M	1	NAG	O7-C7-N2-C2
5	U	1	NAG	C8-C7-N2-C2
5	U	1	NAG	O7-C7-N2-C2
5	c	1	NAG	C8-C7-N2-C2
5	c	1	NAG	O7-C7-N2-C2
7	S	1	NAG	O5-C5-C6-O6
7	a	1	NAG	O5-C5-C6-O6
7	i	1	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
5	e	2	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
5	e	1	NAG	O5-C5-C6-O6
6	Q	3	BMA	O5-C5-C6-O6
6	Y	3	BMA	O5-C5-C6-O6
6	g	3	BMA	O5-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
5	j	2	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6
7	S	5	MAN	O5-C5-C6-O6
7	a	5	MAN	O5-C5-C6-O6
7	i	5	MAN	O5-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
7	a	1	NAG	C4-C5-C6-O6
7	i	1	NAG	C4-C5-C6-O6

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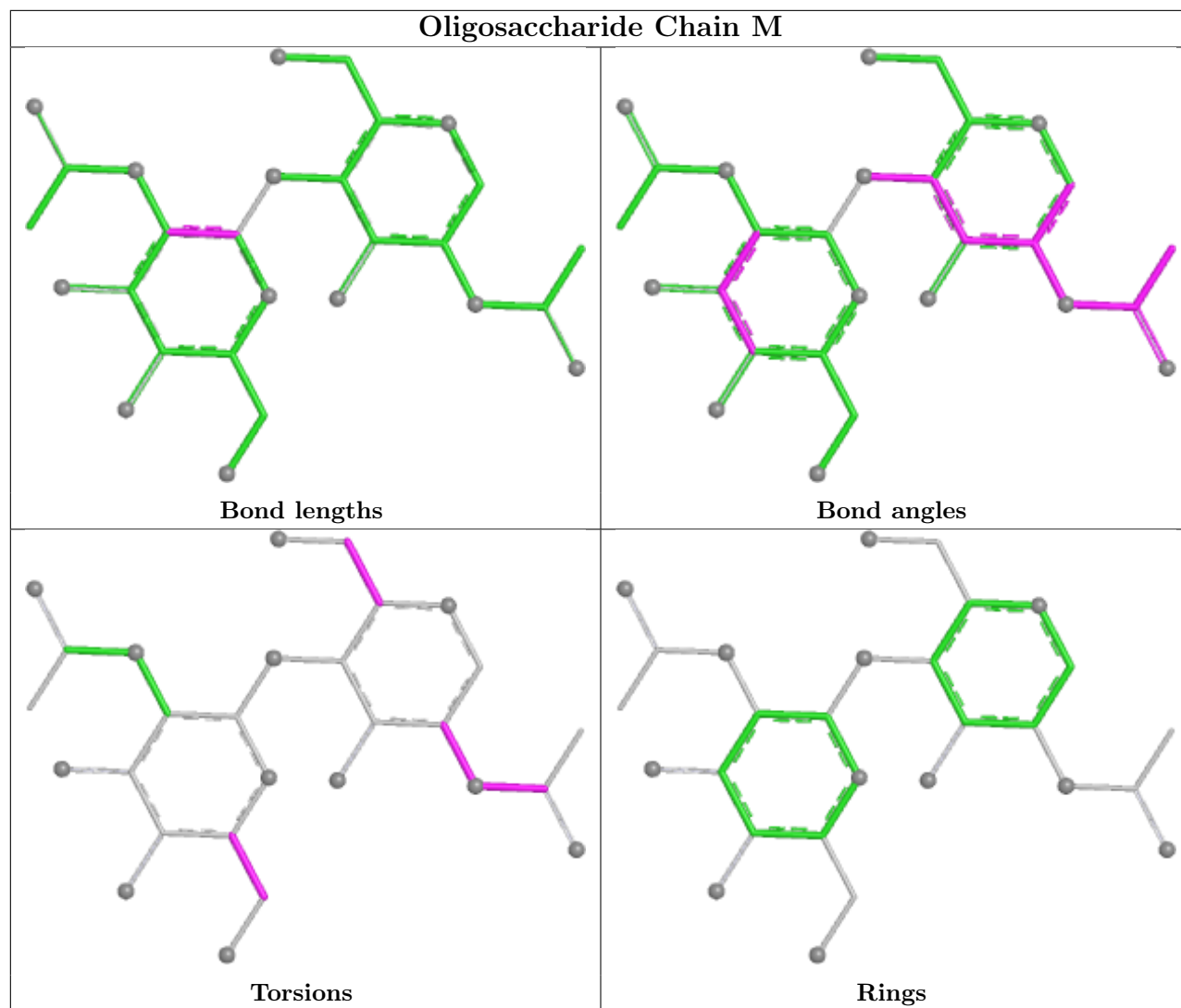
Mol	Chain	Res	Type	Atoms
5	e	2	NAG	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6

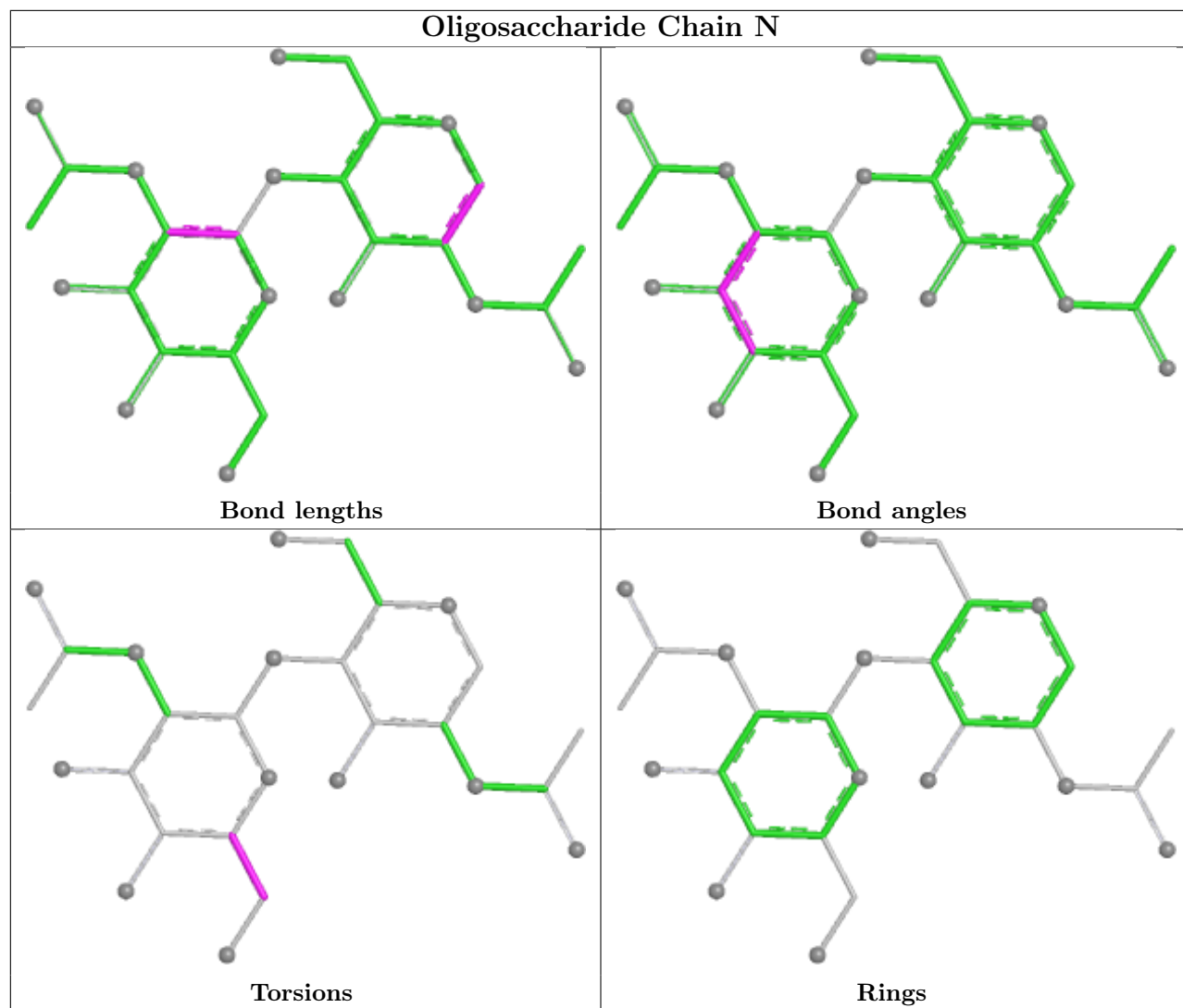
There are no ring outliers.

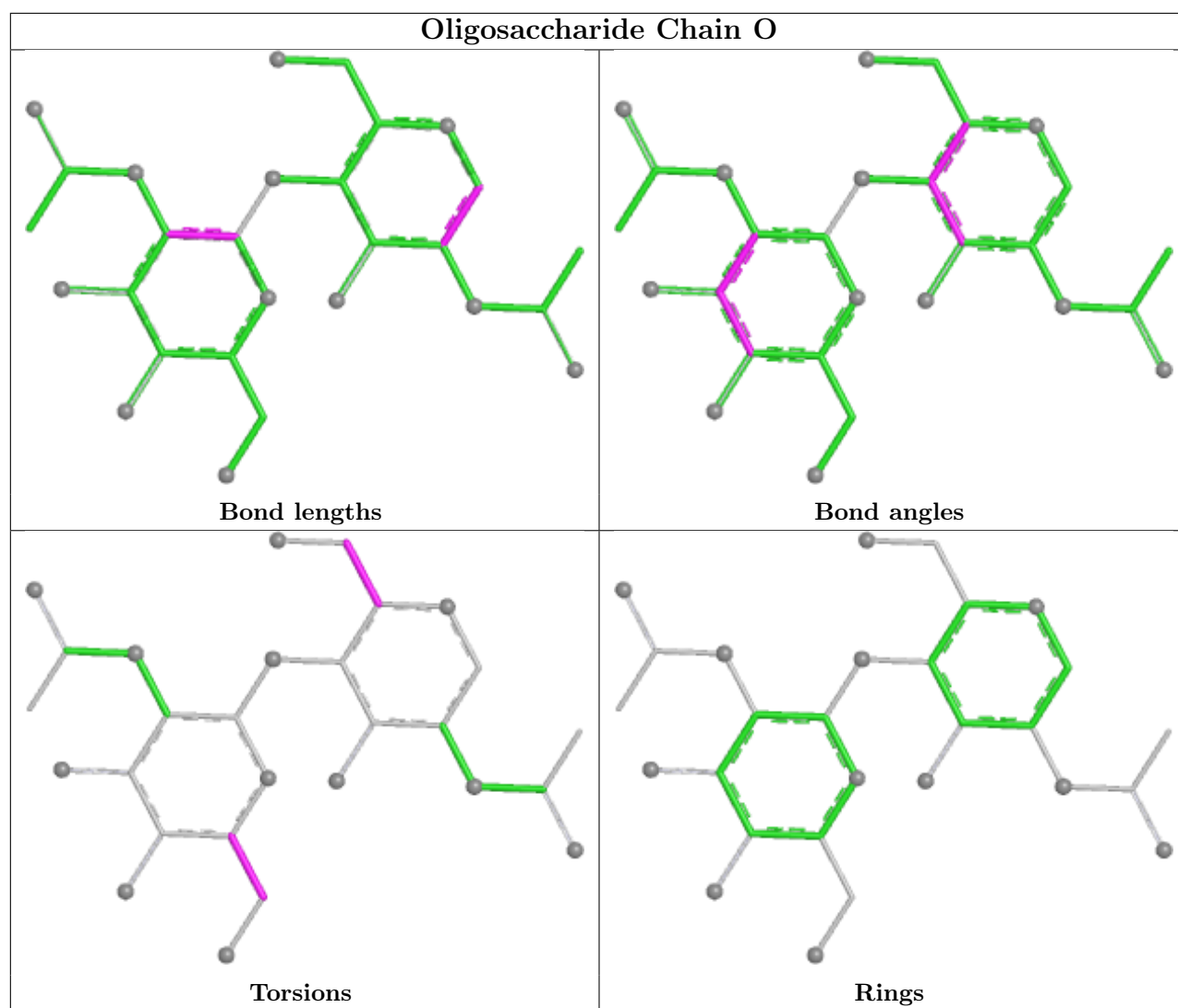
10 monomers are involved in 10 short contacts:

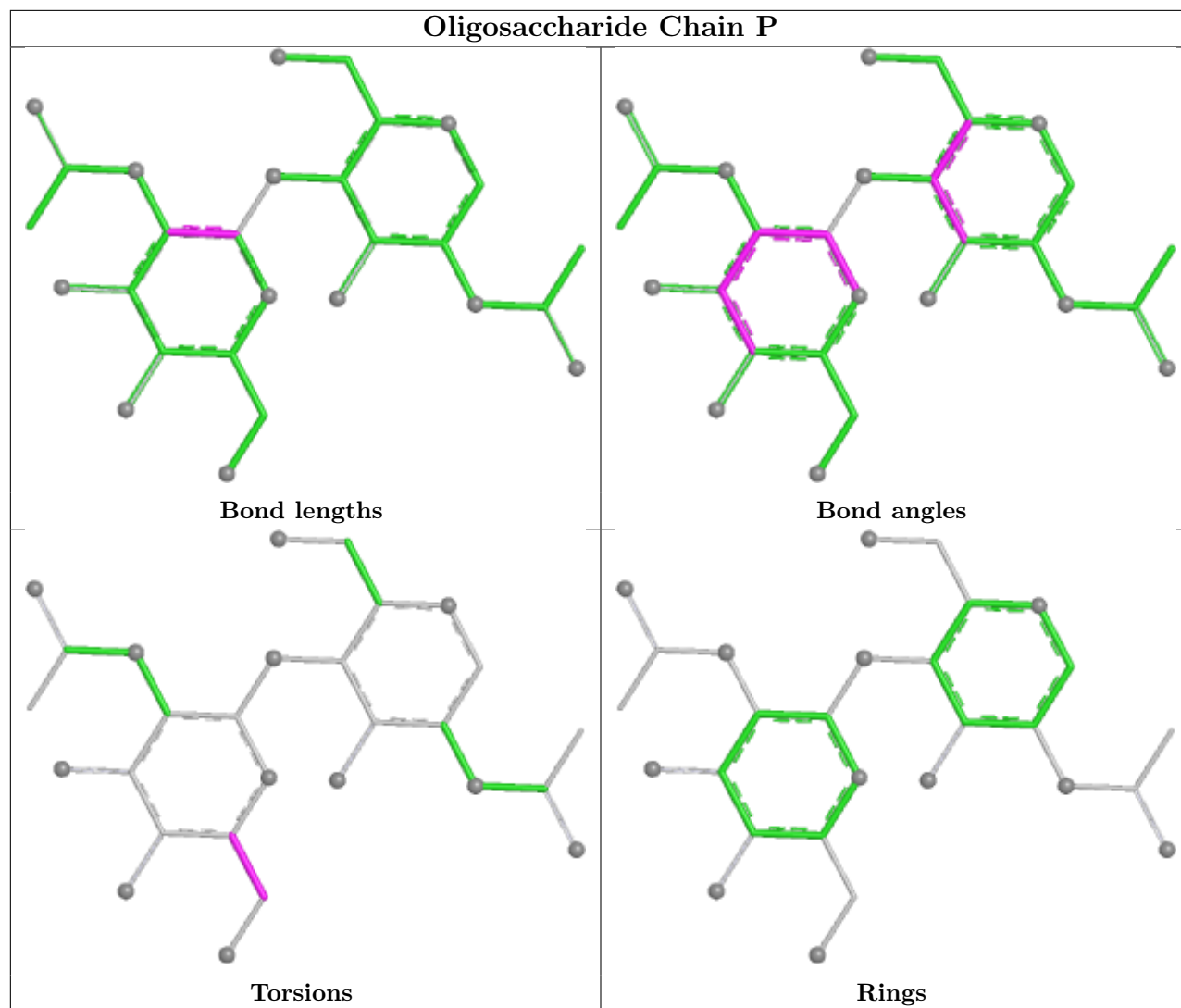
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	2	NAG	1	0
6	Q	1	NAG	1	0
5	M	2	NAG	1	0
6	g	3	BMA	1	0
5	N	1	NAG	1	0
5	c	2	NAG	1	0
5	d	1	NAG	1	0
5	V	1	NAG	1	0
6	g	1	NAG	1	0
6	Y	1	NAG	1	0

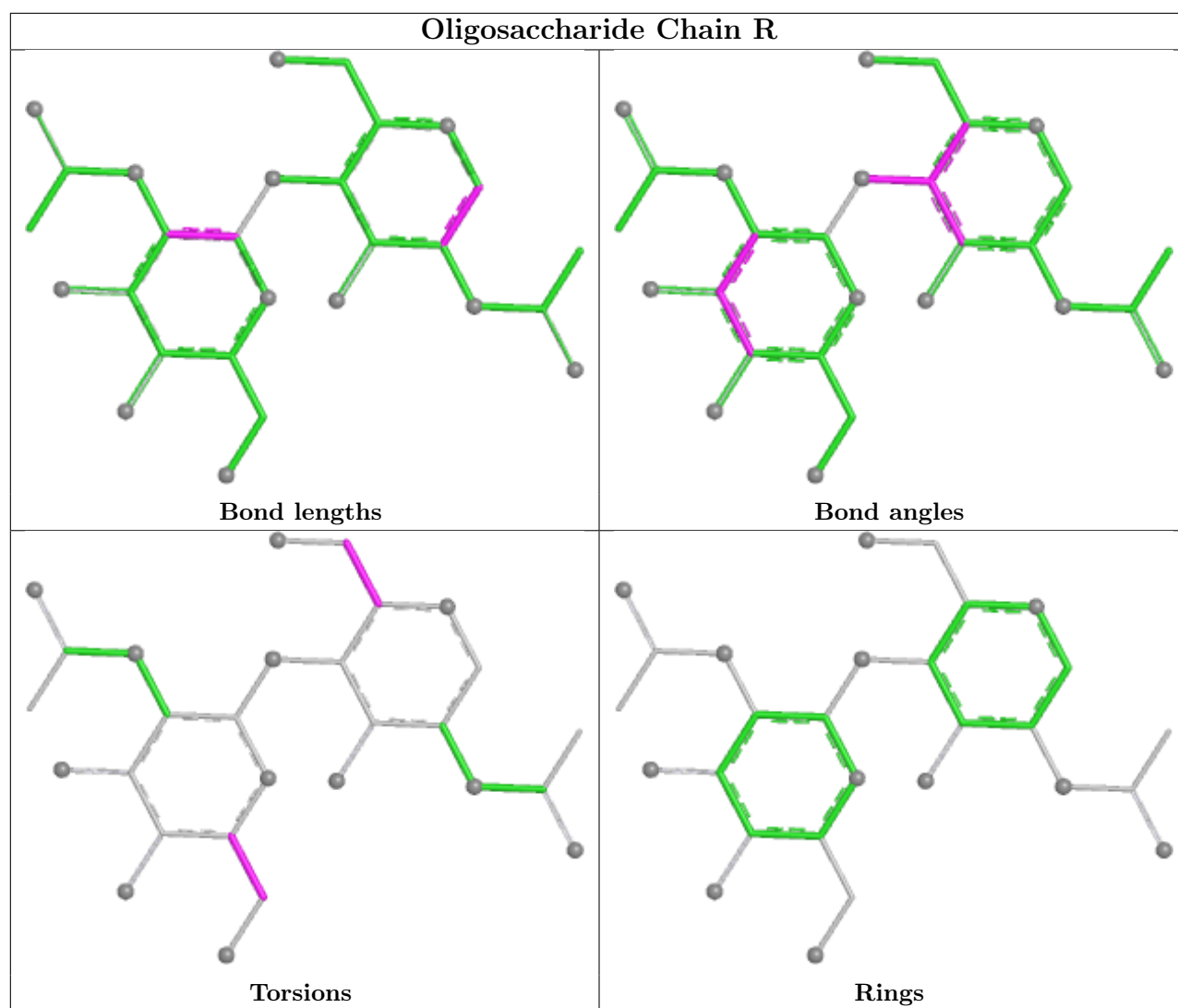
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

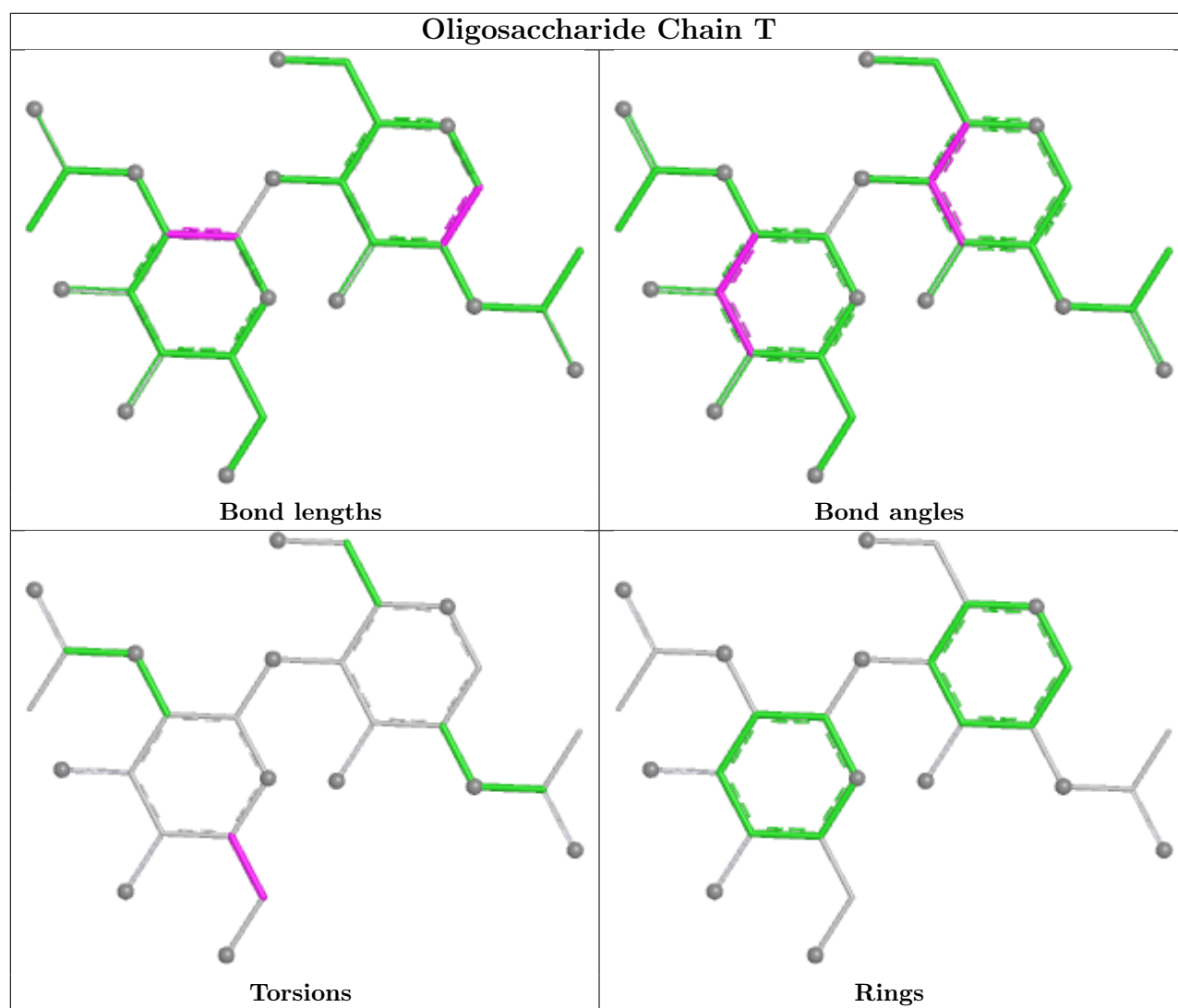


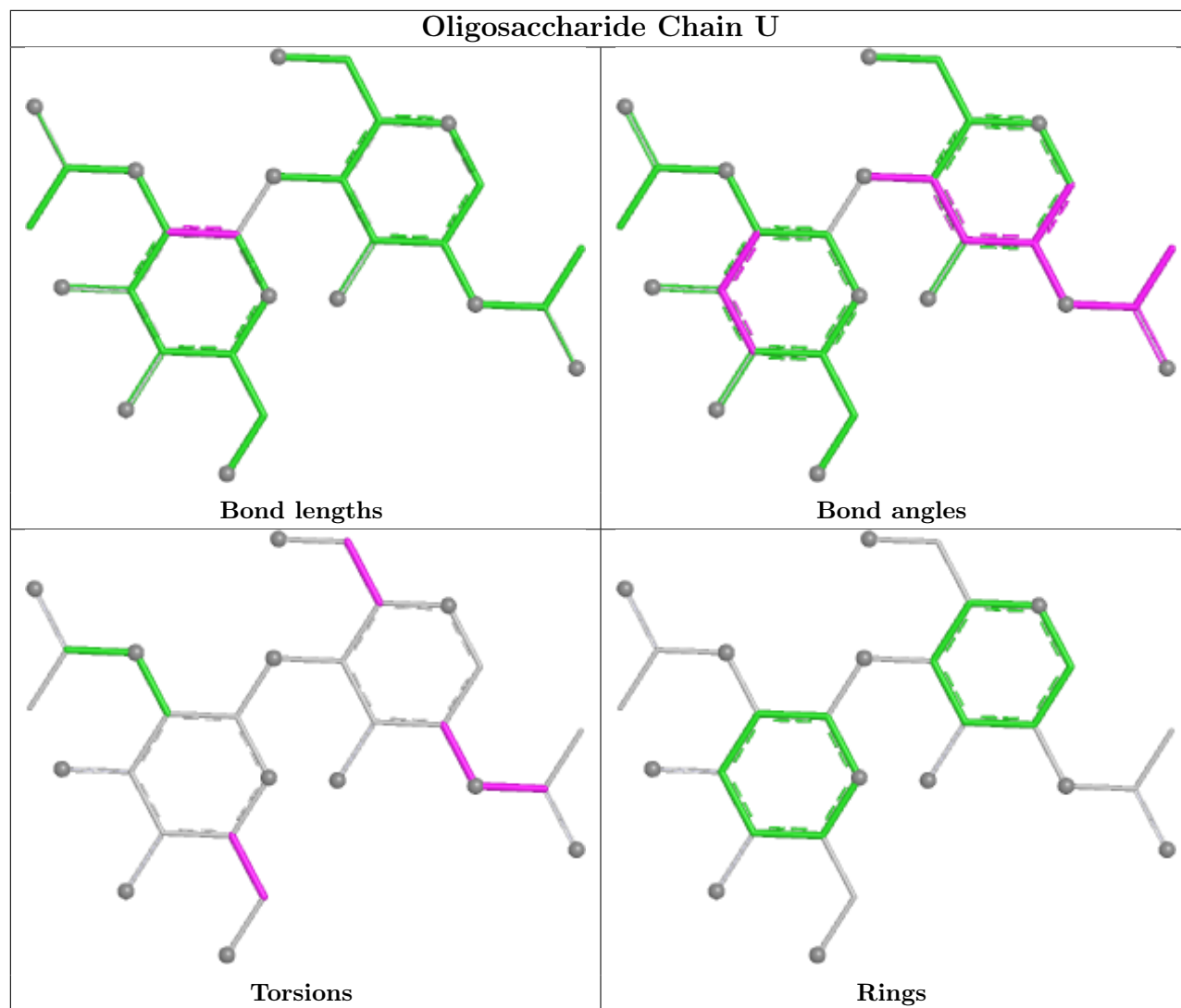


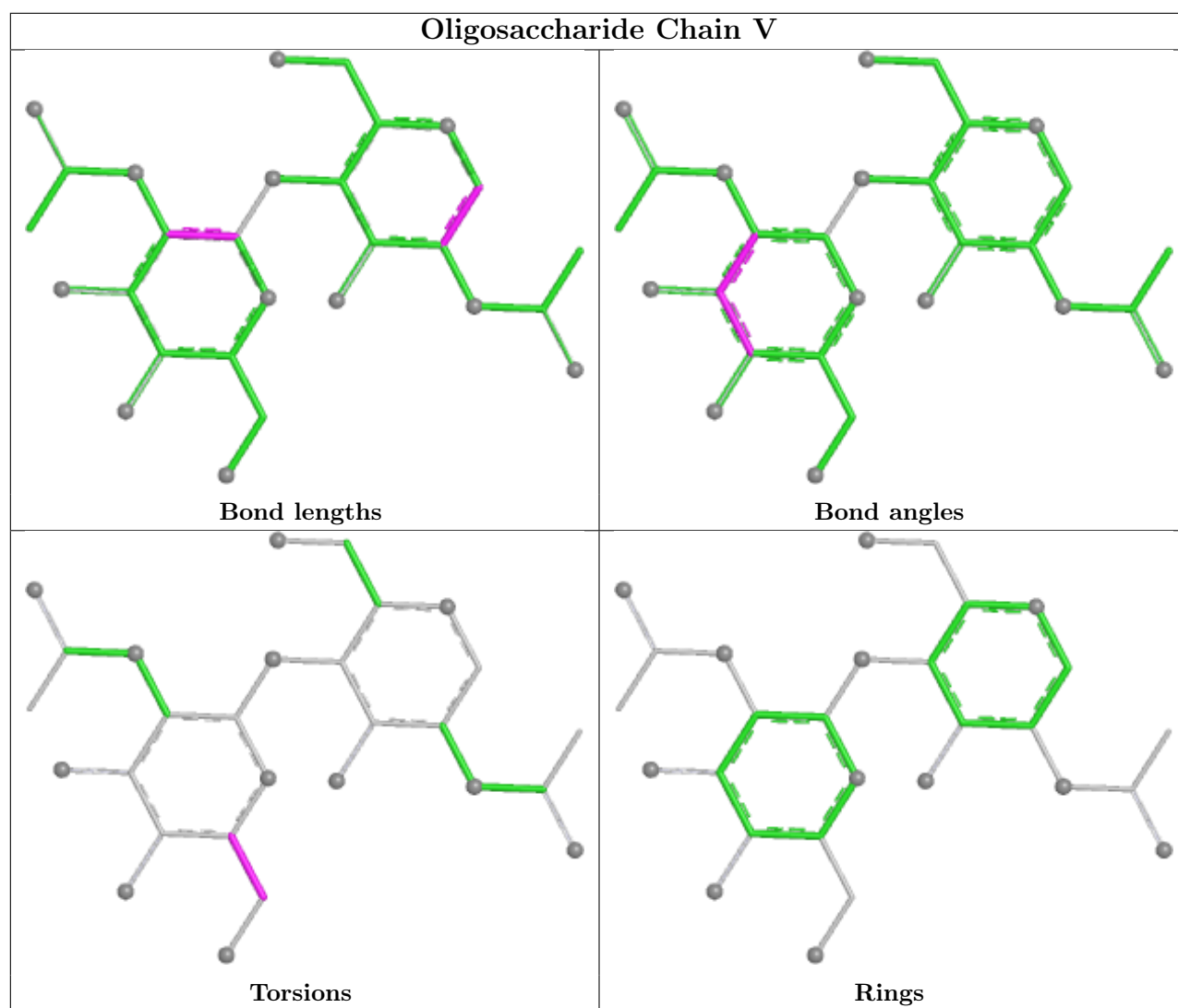


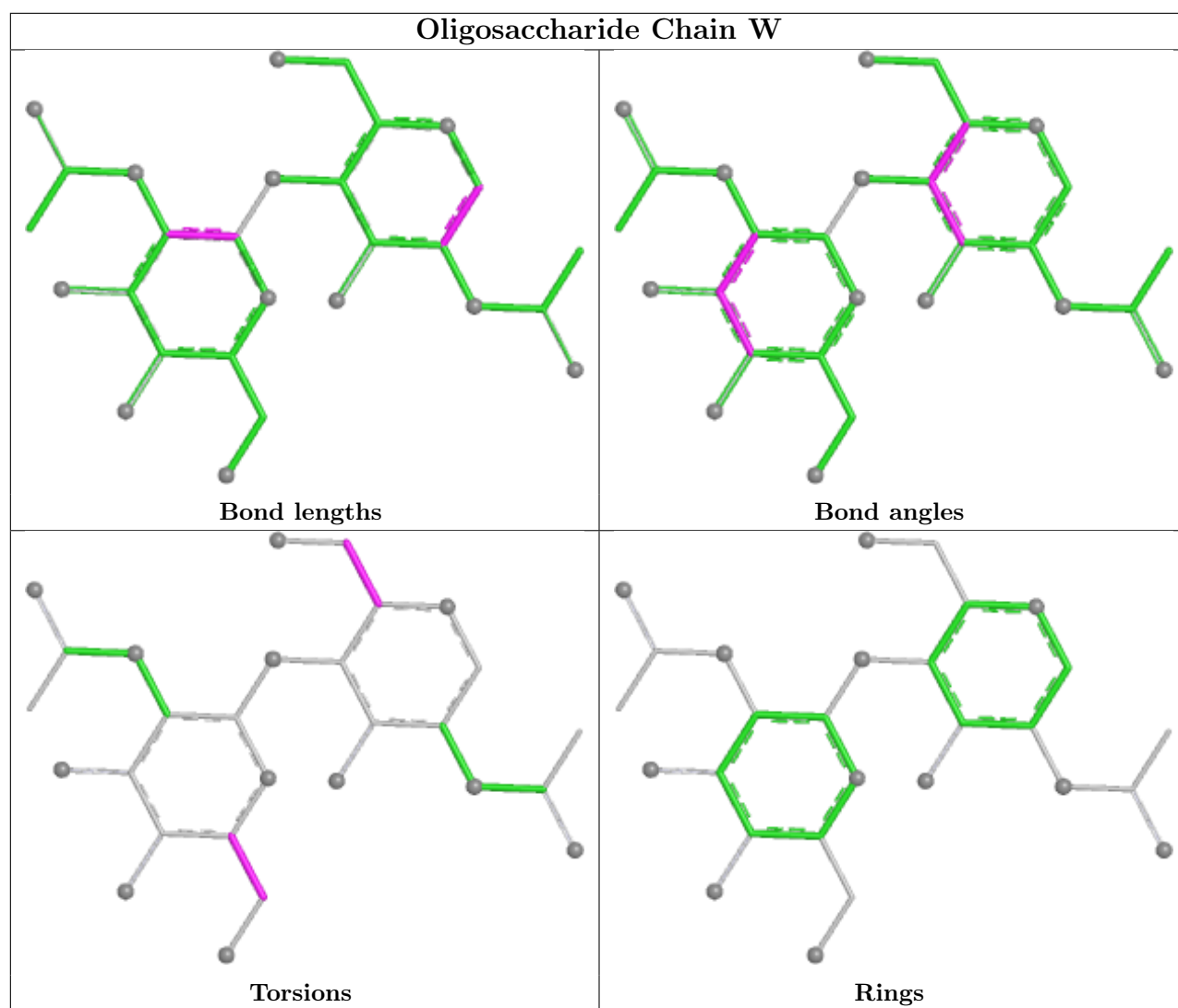


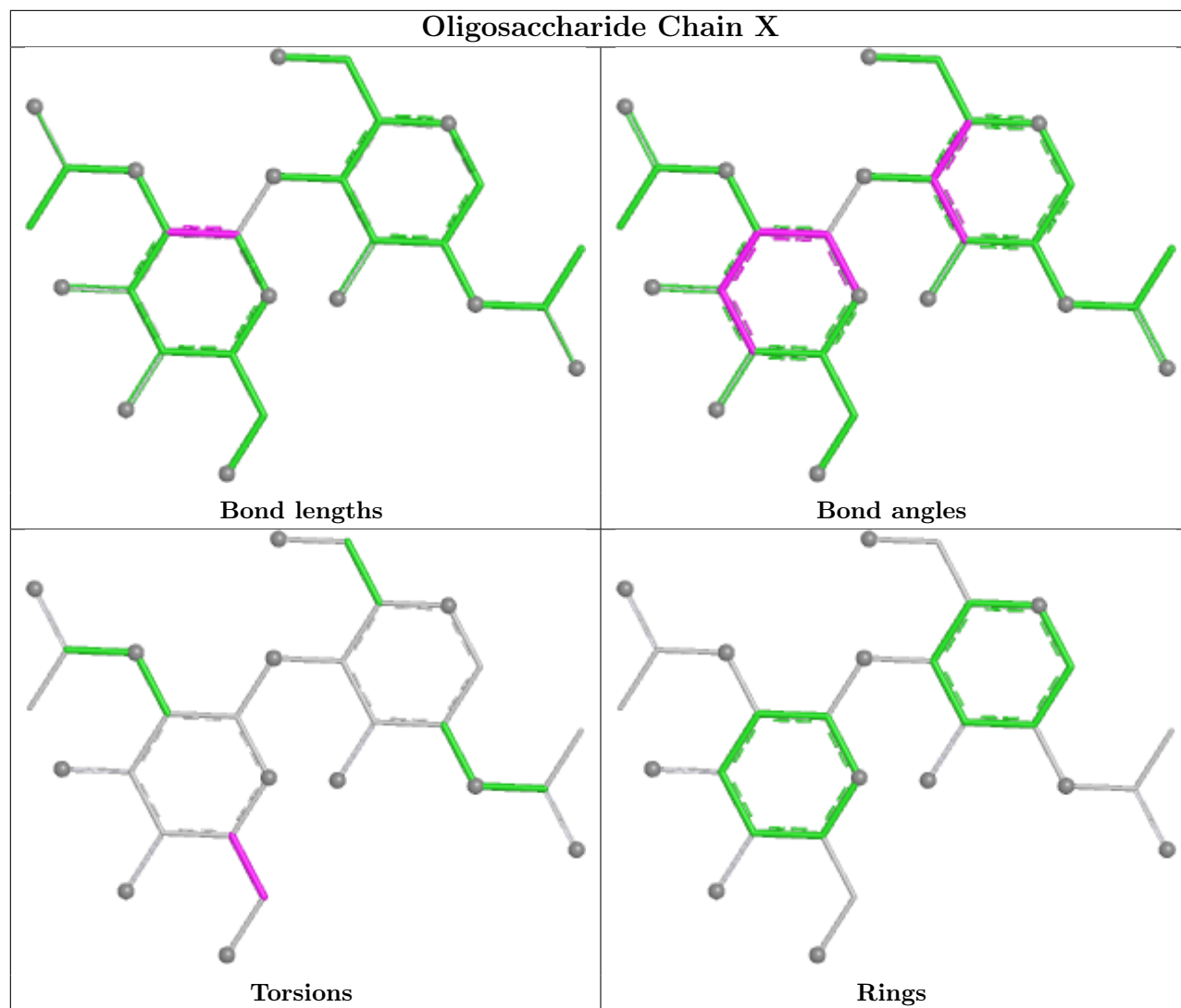


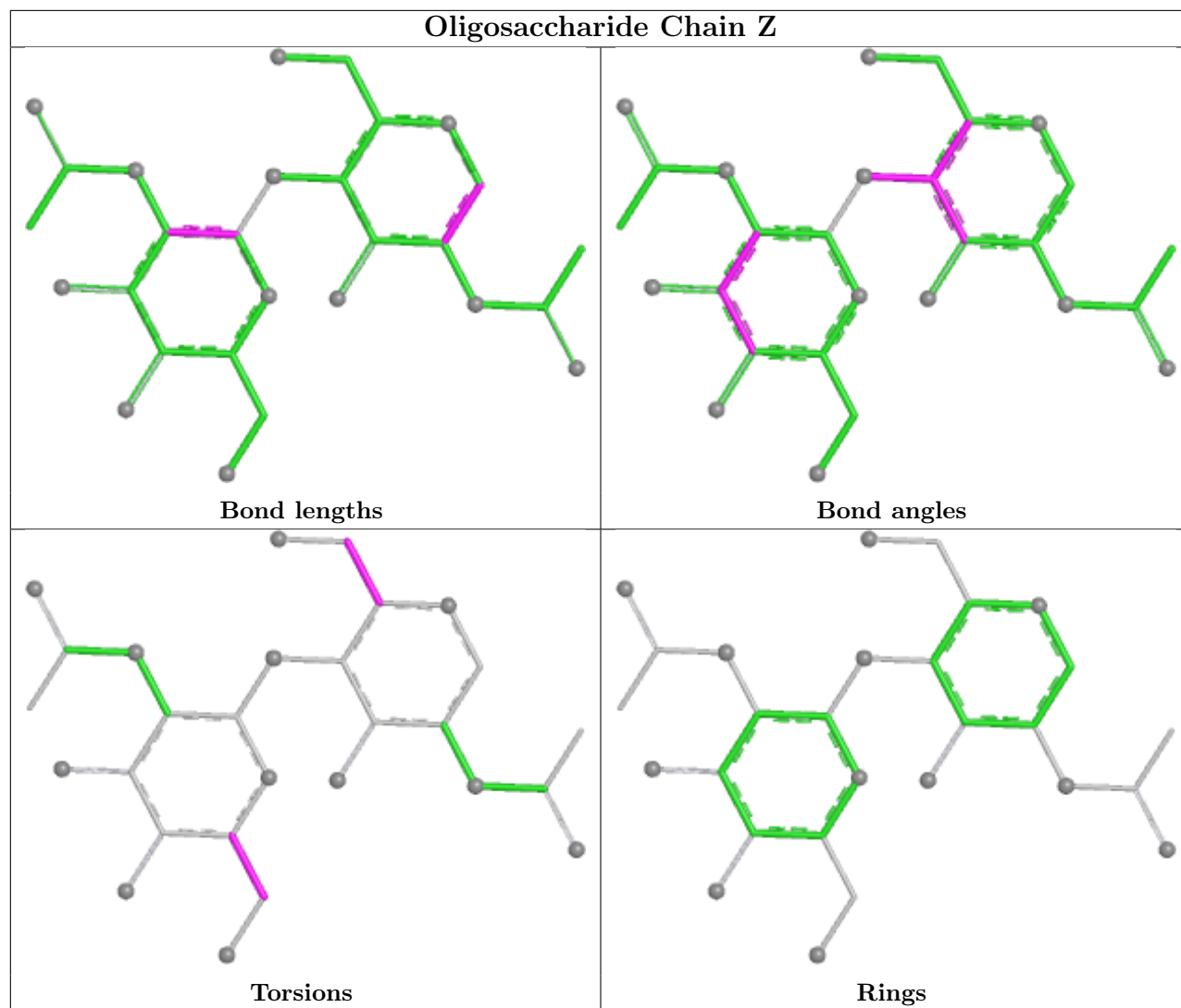


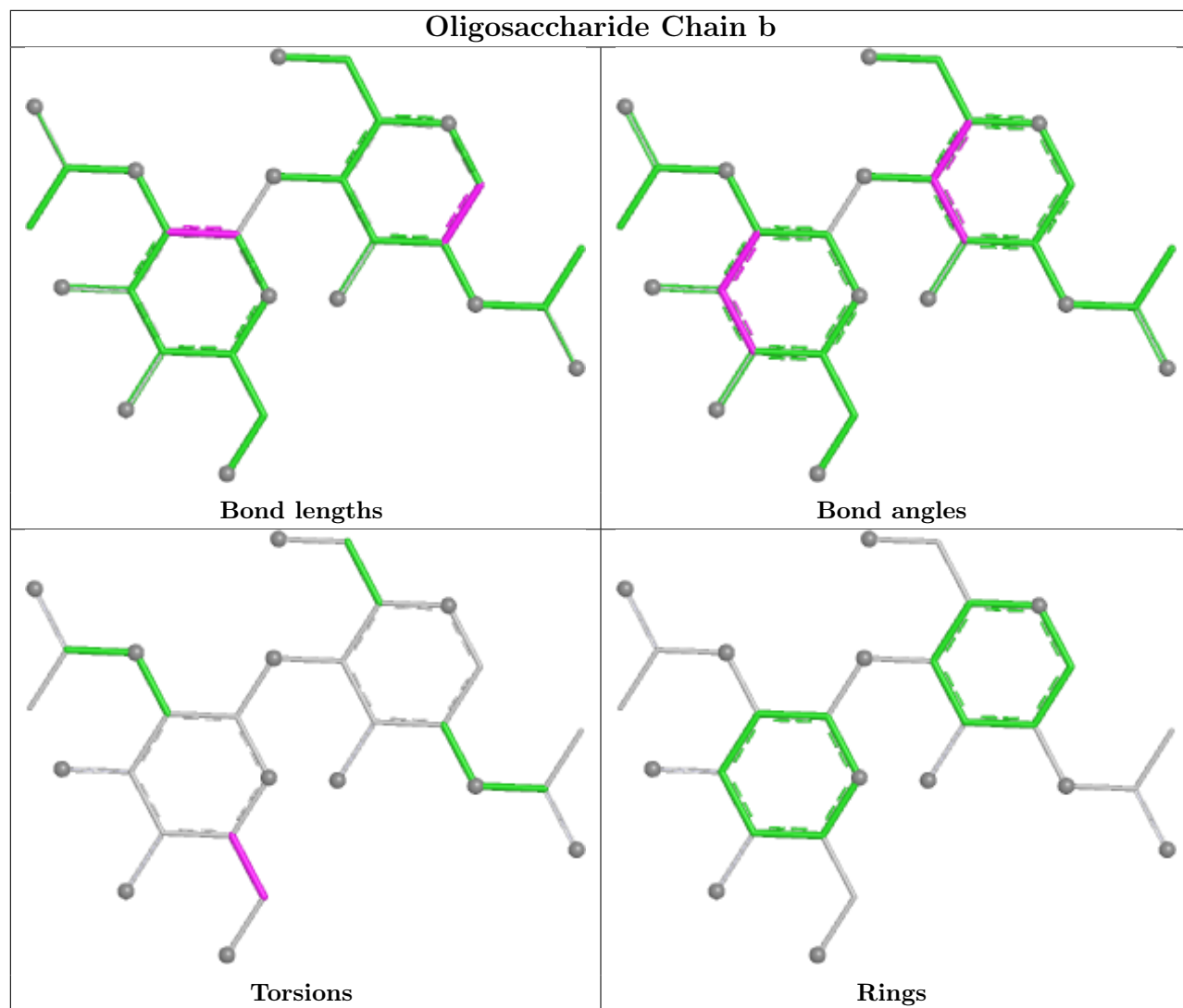


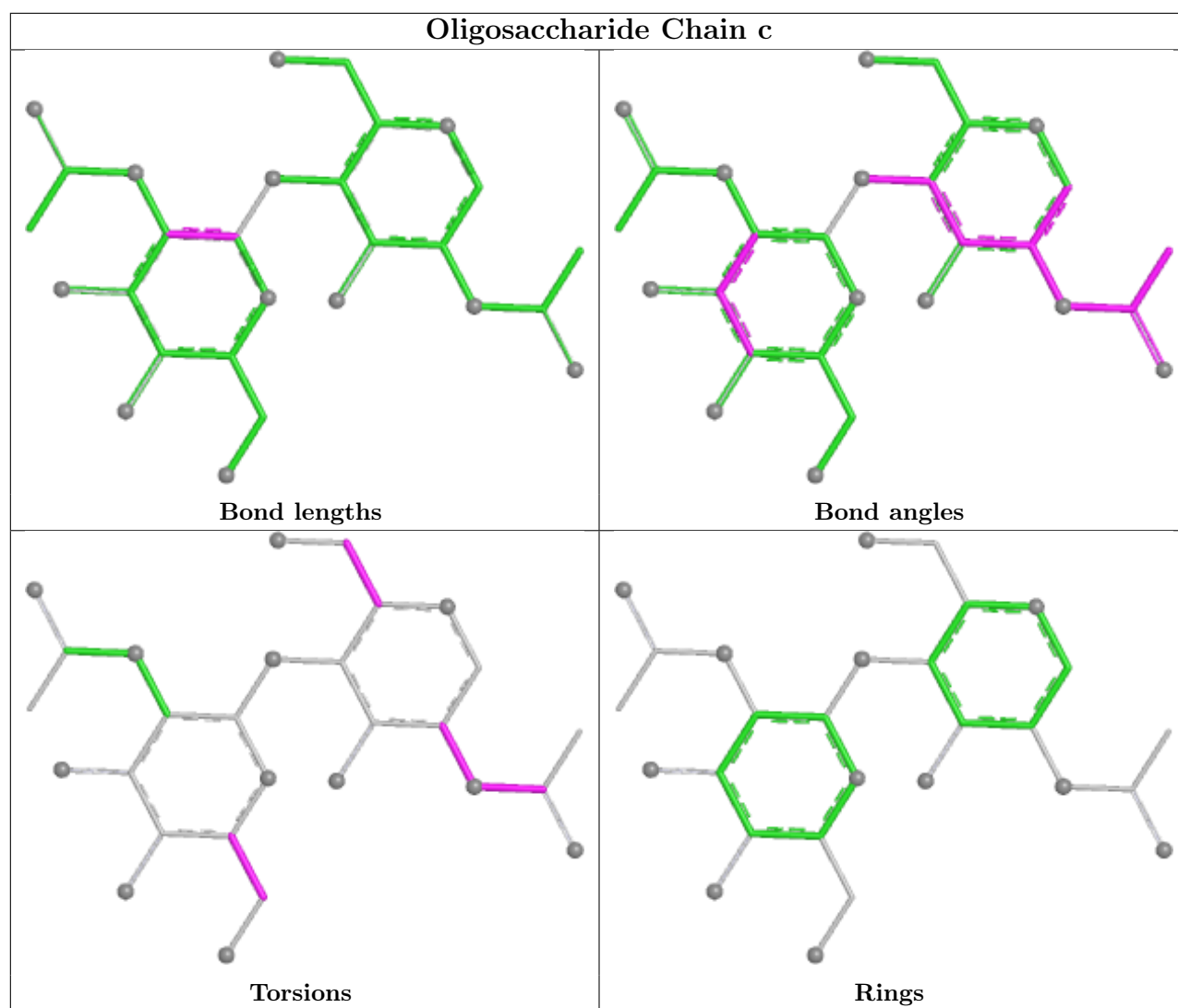


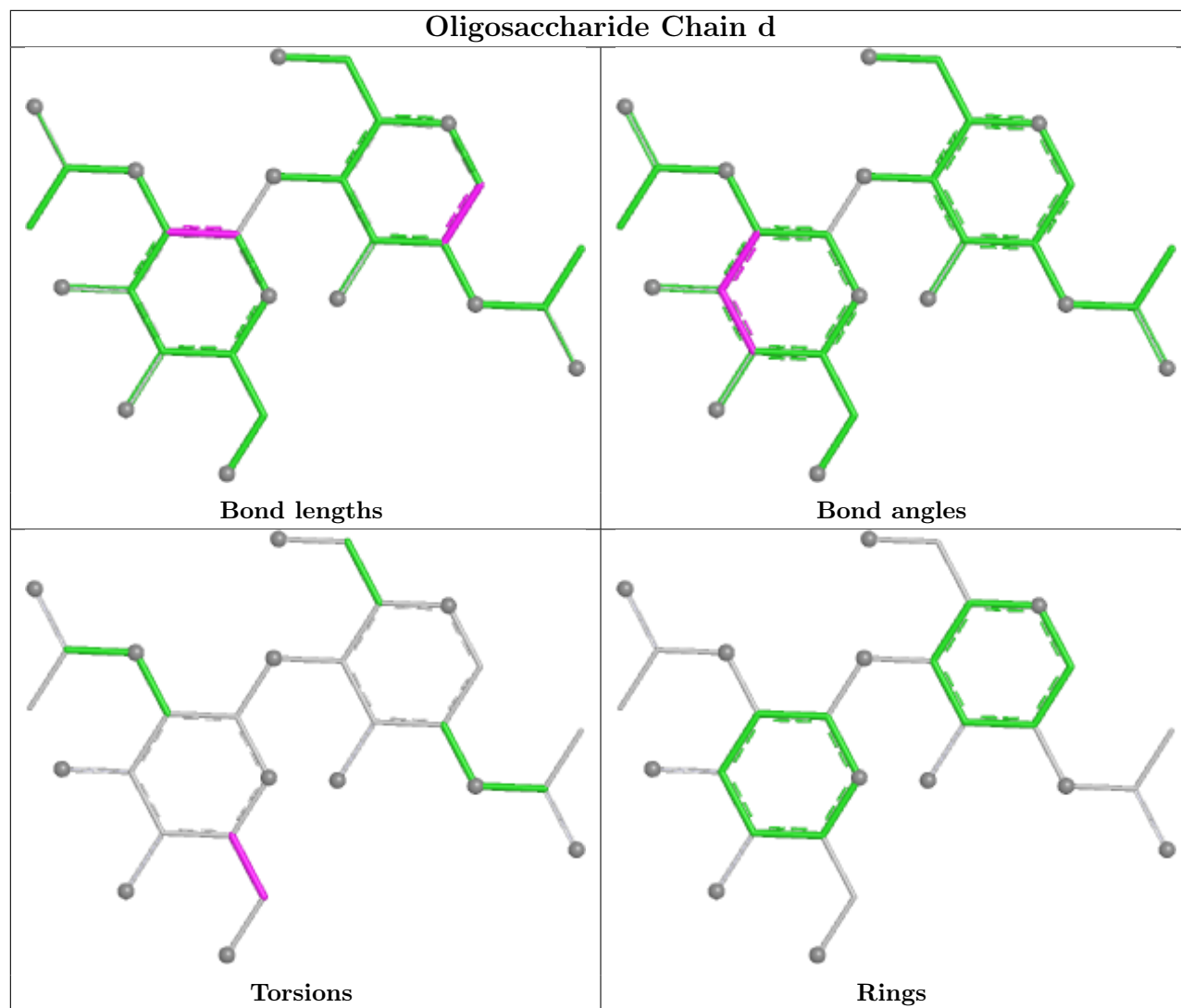


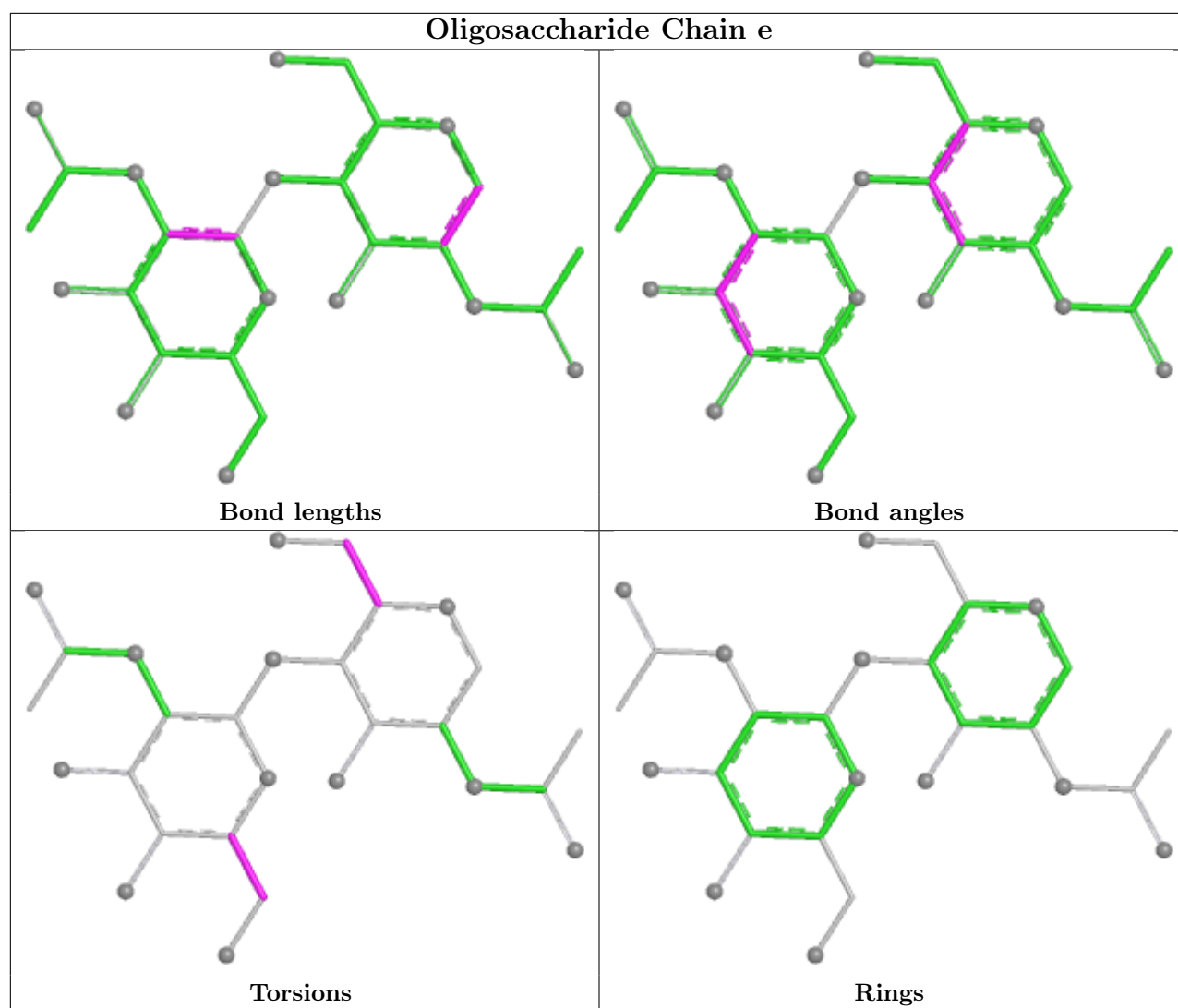


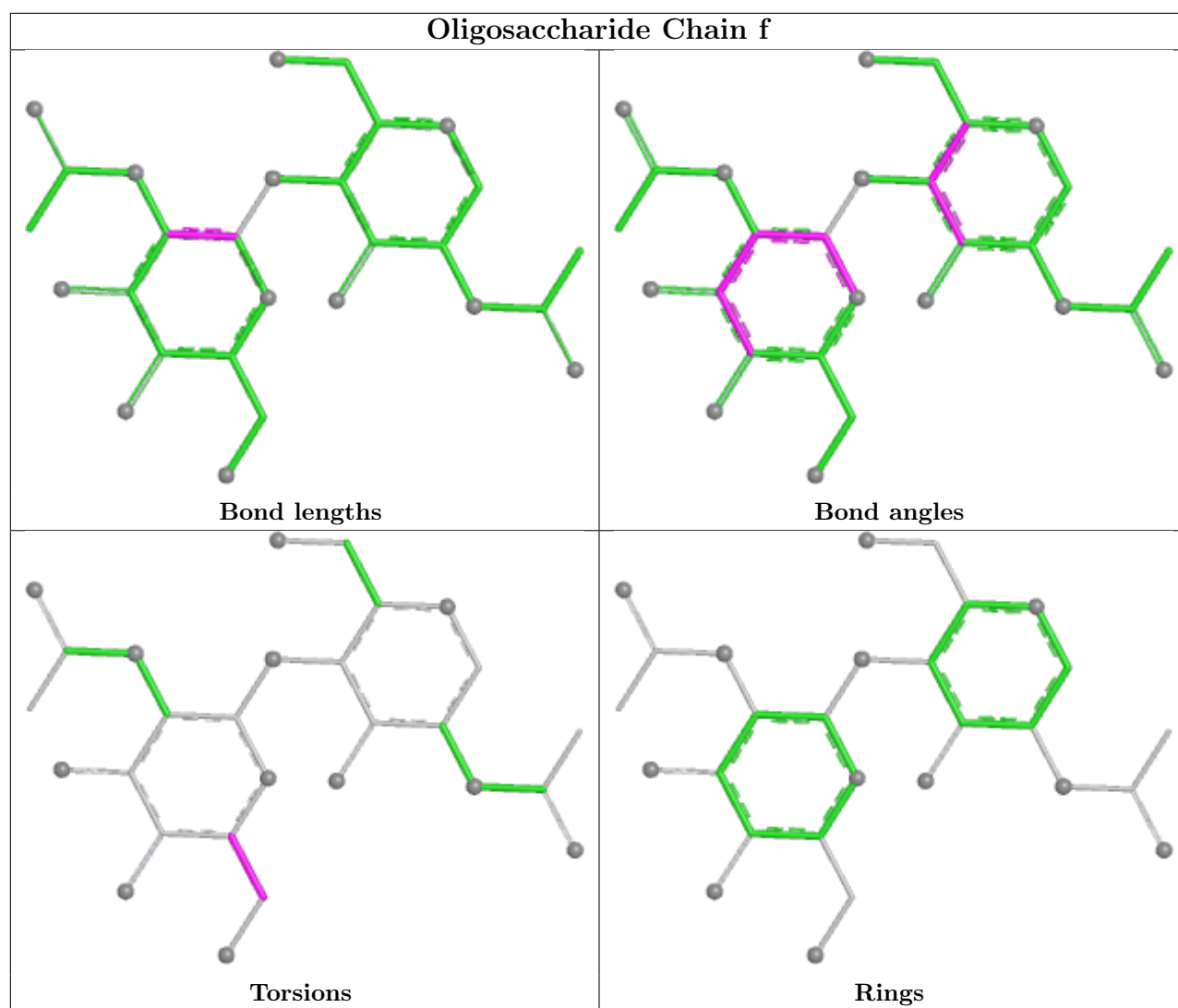


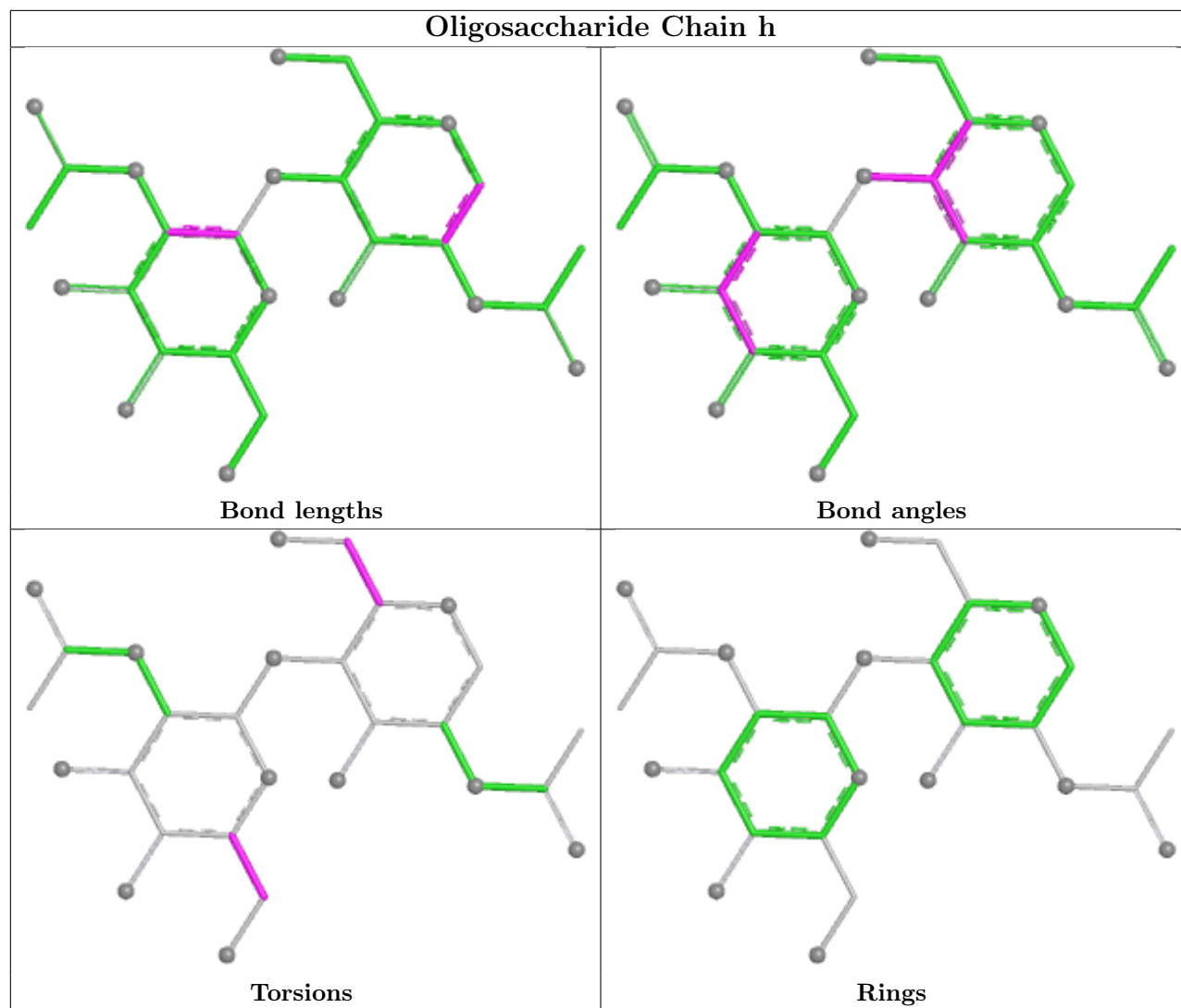


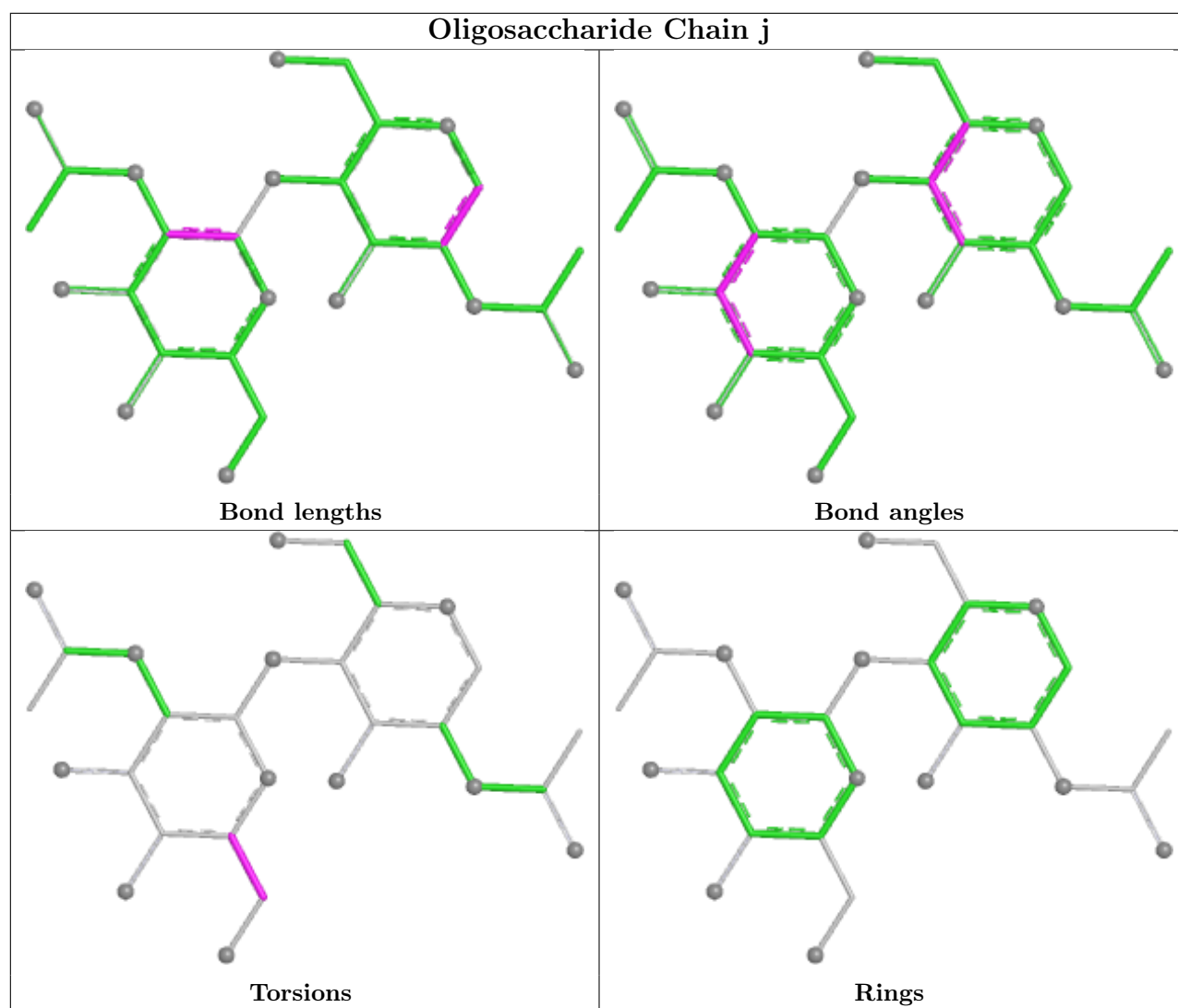


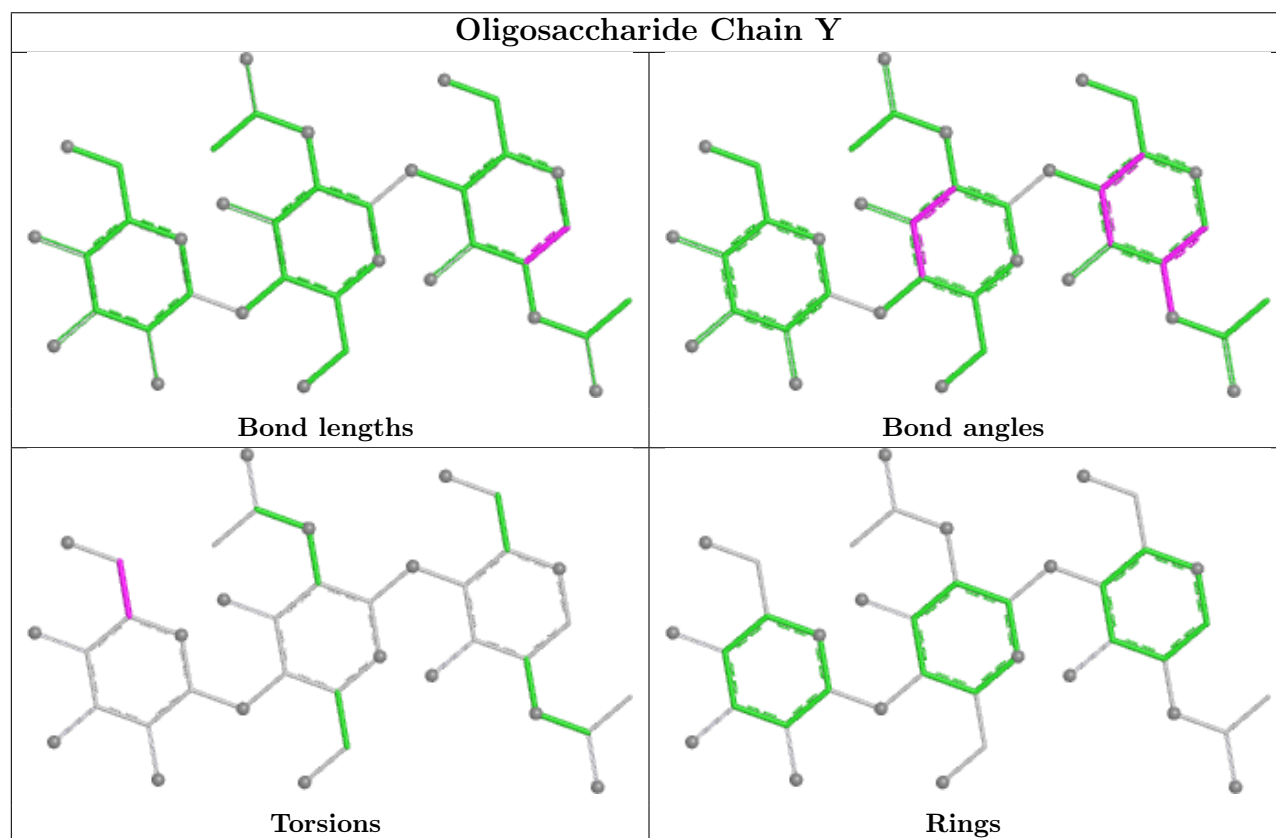
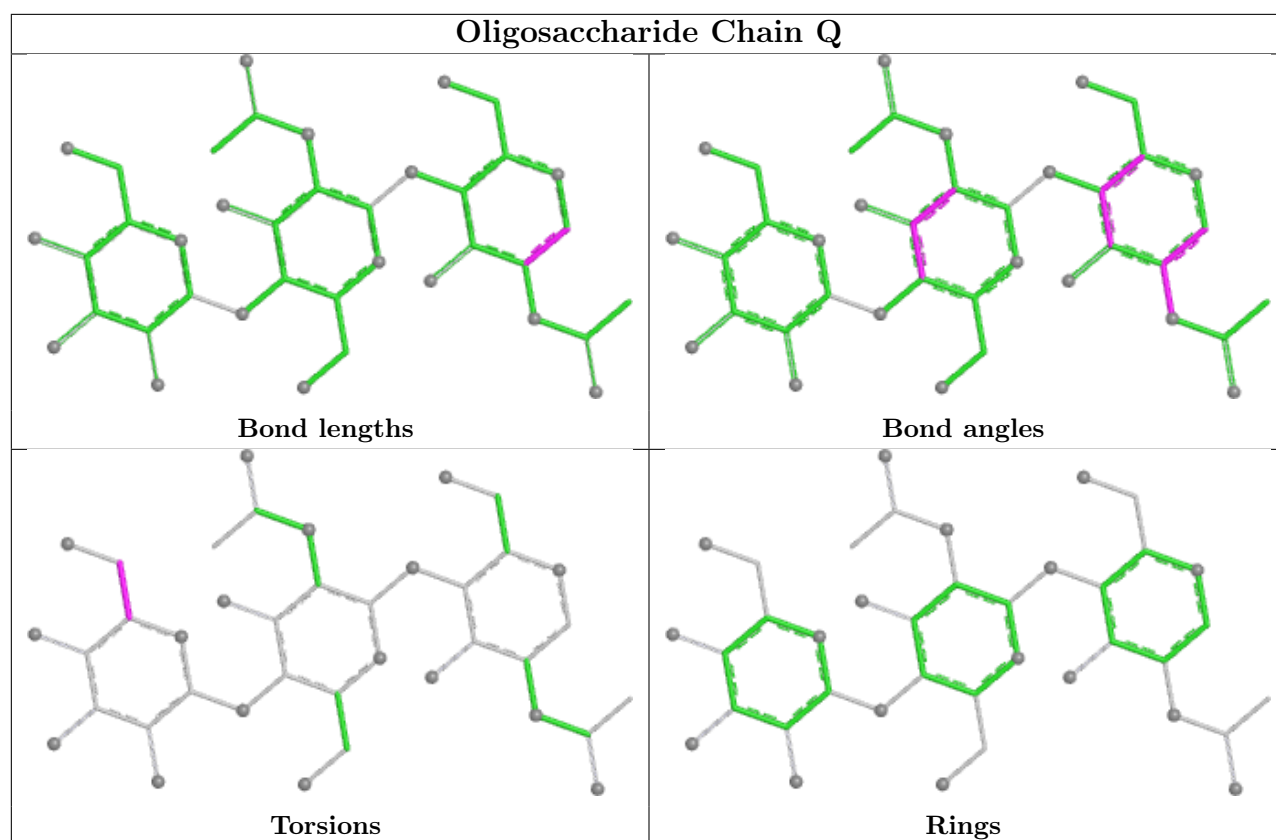


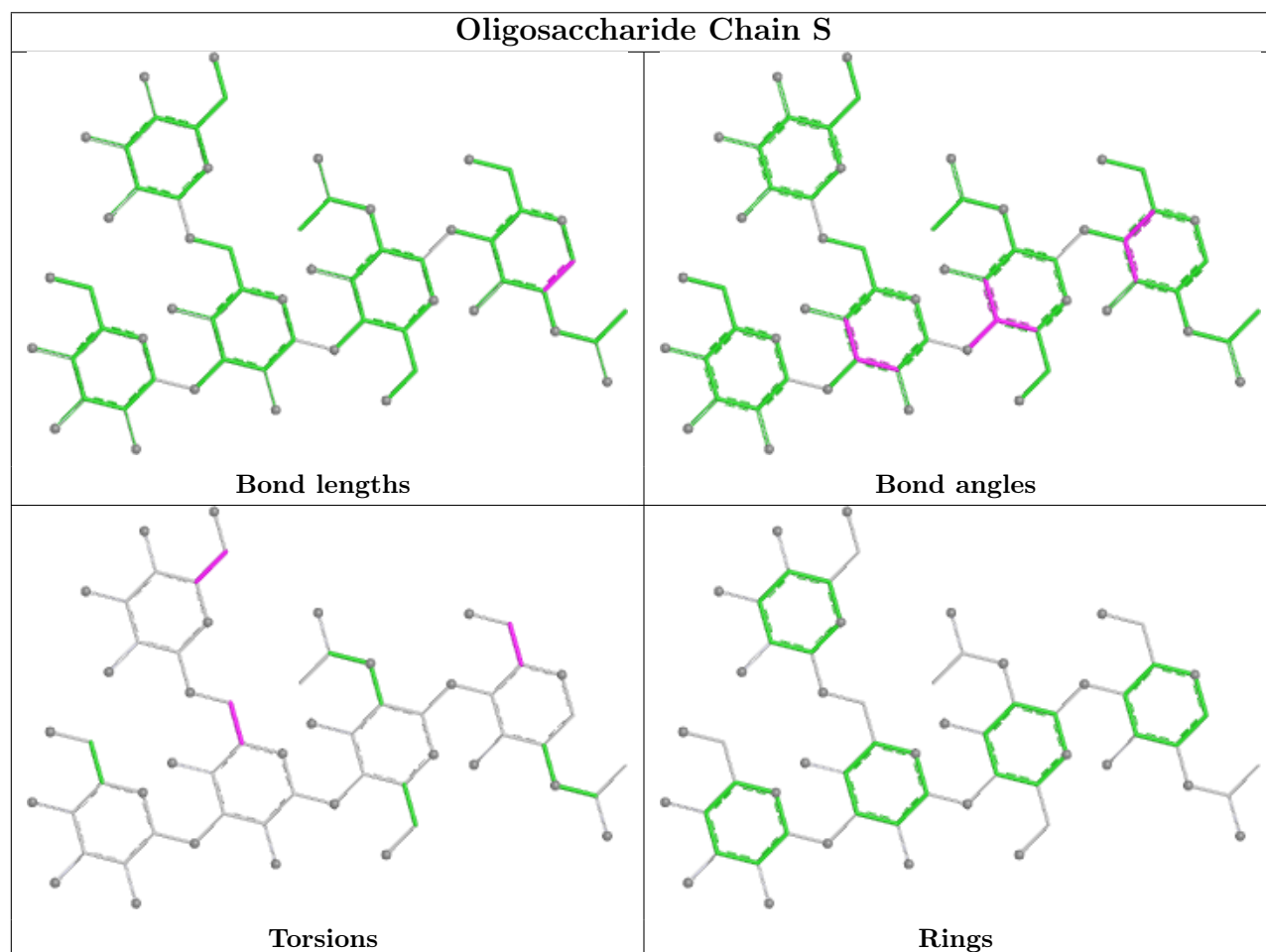
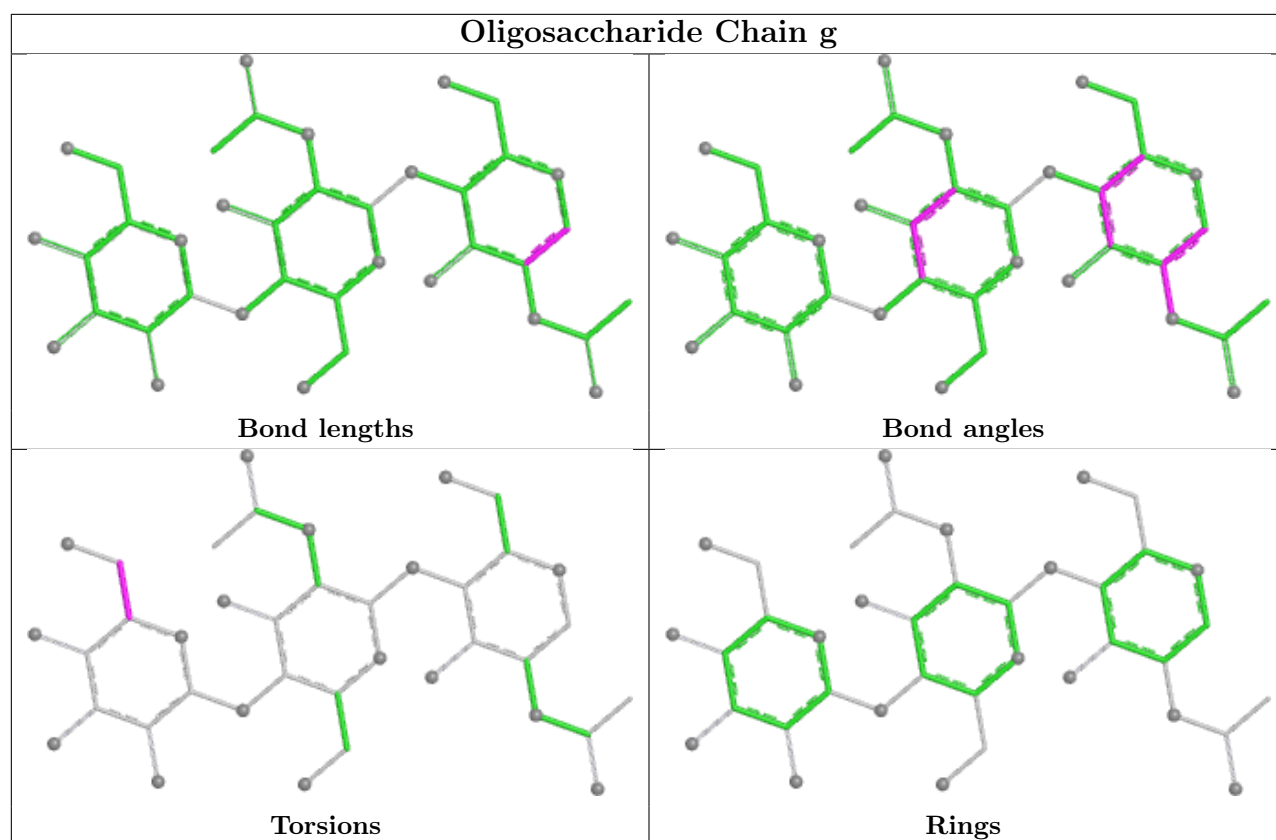


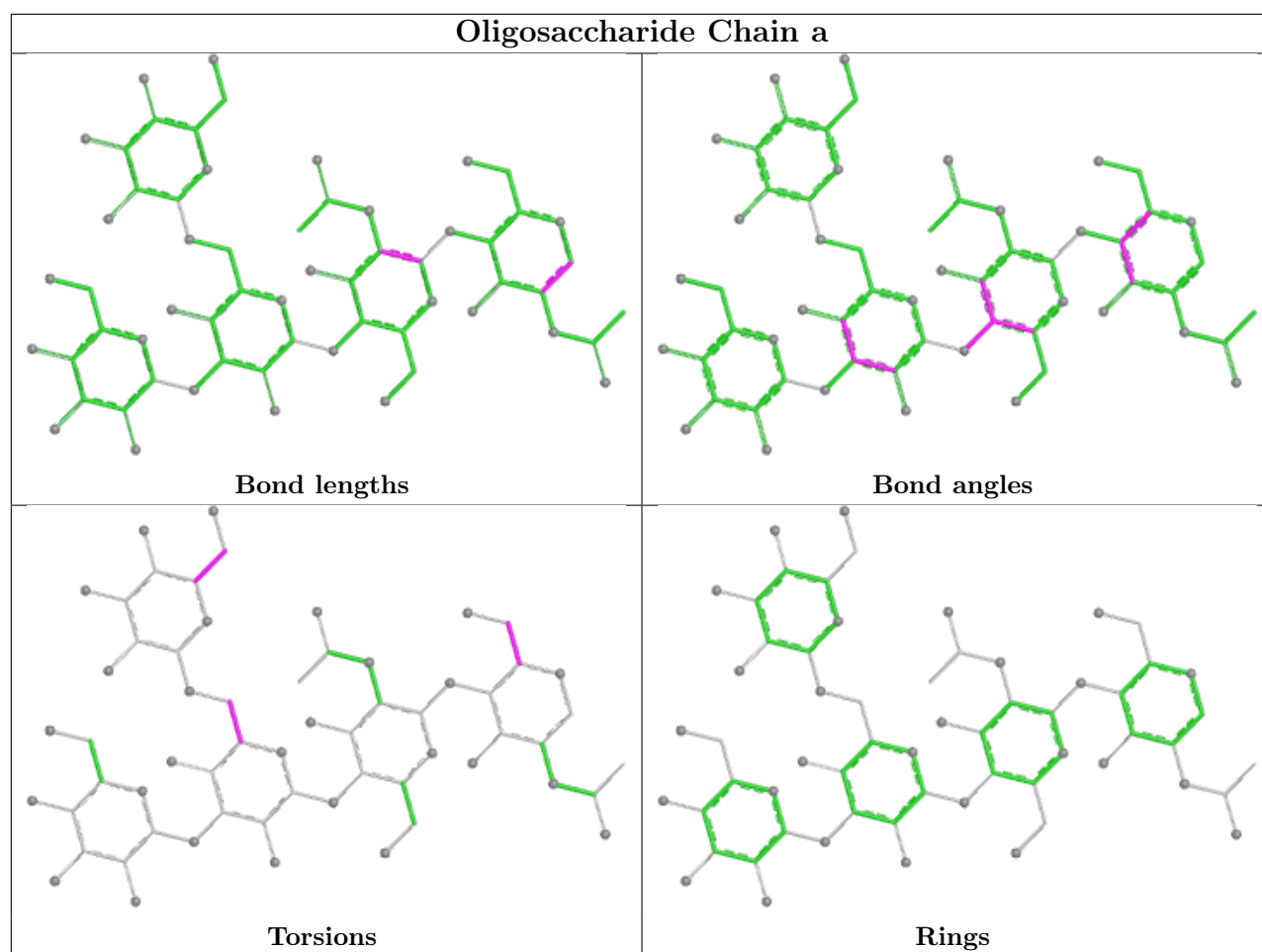


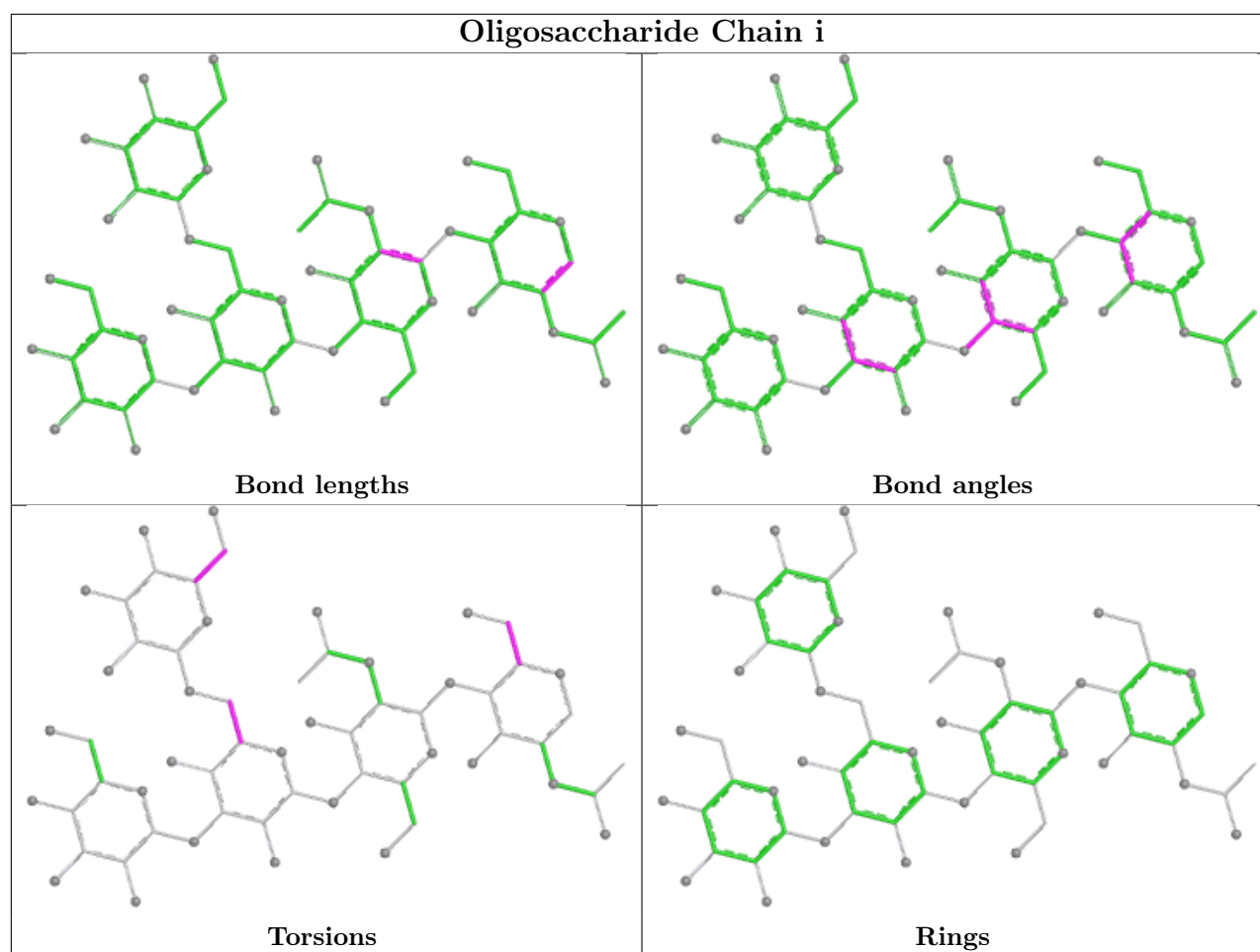












5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	B	801	2	14,14,15	0.76	1 (7%)	17,19,21	0.74	0
8	NAG	I	1401	1	14,14,15	0.88	1 (7%)	17,19,21	0.96	1 (5%)
8	NAG	F	803	2	14,14,15	0.92	1 (7%)	17,19,21	1.00	1 (5%)
8	NAG	F	807	2	14,14,15	0.97	1 (7%)	17,19,21	0.78	1 (5%)
8	NAG	E	1401	1	14,14,15	0.88	1 (7%)	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	J	801	2	14,14,15	0.76	1 (7%)	17,19,21	0.74	0
8	NAG	A	1401	1	14,14,15	0.87	1 (7%)	17,19,21	0.96	1 (5%)
8	NAG	J	802	2	14,14,15	0.96	1 (7%)	17,19,21	1.04	1 (5%)
8	NAG	J	803	2	14,14,15	0.91	1 (7%)	17,19,21	1.00	1 (5%)
8	NAG	F	817	2	14,14,15	1.06	1 (7%)	17,19,21	0.81	1 (5%)
8	NAG	B	807	2	14,14,15	0.97	1 (7%)	17,19,21	0.79	1 (5%)
8	NAG	J	817	2	14,14,15	1.05	1 (7%)	17,19,21	0.81	1 (5%)
8	NAG	F	801	2	14,14,15	0.76	1 (7%)	17,19,21	0.75	1 (5%)
8	NAG	B	802	2	14,14,15	0.95	1 (7%)	17,19,21	1.04	1 (5%)
8	NAG	F	802	2	14,14,15	0.96	1 (7%)	17,19,21	1.03	1 (5%)
8	NAG	B	803	2	14,14,15	0.92	1 (7%)	17,19,21	1.00	1 (5%)
8	NAG	B	817	2	14,14,15	1.06	1 (7%)	17,19,21	0.81	1 (5%)
8	NAG	J	807	2	14,14,15	0.98	1 (7%)	17,19,21	0.79	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	801	2	-	1/6/23/26	0/1/1/1
8	NAG	I	1401	1	-	1/6/23/26	0/1/1/1
8	NAG	F	803	2	-	1/6/23/26	0/1/1/1
8	NAG	F	807	2	-	1/6/23/26	0/1/1/1
8	NAG	E	1401	1	-	1/6/23/26	0/1/1/1
8	NAG	J	801	2	-	1/6/23/26	0/1/1/1
8	NAG	A	1401	1	-	1/6/23/26	0/1/1/1
8	NAG	J	802	2	-	1/6/23/26	0/1/1/1
8	NAG	J	803	2	-	1/6/23/26	0/1/1/1
8	NAG	F	817	2	-	1/6/23/26	0/1/1/1
8	NAG	B	807	2	-	1/6/23/26	0/1/1/1
8	NAG	J	817	2	-	1/6/23/26	0/1/1/1
8	NAG	F	801	2	-	1/6/23/26	0/1/1/1
8	NAG	B	802	2	-	1/6/23/26	0/1/1/1
8	NAG	F	802	2	-	1/6/23/26	0/1/1/1
8	NAG	B	803	2	-	1/6/23/26	0/1/1/1
8	NAG	B	817	2	-	1/6/23/26	0/1/1/1
8	NAG	J	807	2	-	1/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	817	NAG	C1-C2	3.33	1.56	1.52
8	J	817	NAG	C1-C2	3.33	1.56	1.52
8	F	817	NAG	C1-C2	3.33	1.56	1.52
8	J	807	NAG	C1-C2	3.32	1.56	1.52
8	B	807	NAG	C1-C2	3.29	1.56	1.52
8	F	807	NAG	C1-C2	3.29	1.56	1.52
8	J	802	NAG	C1-C2	3.11	1.56	1.52
8	F	802	NAG	C1-C2	3.10	1.56	1.52
8	B	802	NAG	C1-C2	3.08	1.56	1.52
8	B	803	NAG	C1-C2	3.05	1.56	1.52
8	F	803	NAG	C1-C2	3.04	1.56	1.52
8	J	803	NAG	C1-C2	3.03	1.56	1.52
8	E	1401	NAG	C1-C2	2.77	1.56	1.52
8	I	1401	NAG	C1-C2	2.76	1.56	1.52
8	A	1401	NAG	C1-C2	2.74	1.56	1.52
8	J	801	NAG	C1-C2	2.52	1.55	1.52
8	B	801	NAG	C1-C2	2.51	1.55	1.52
8	F	801	NAG	C1-C2	2.51	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	803	NAG	C4-C3-C2	-2.89	106.78	111.02
8	B	803	NAG	C4-C3-C2	-2.89	106.78	111.02
8	A	1401	NAG	C4-C3-C2	-2.88	106.79	111.02
8	J	803	NAG	C4-C3-C2	-2.88	106.80	111.02
8	E	1401	NAG	C4-C3-C2	-2.87	106.81	111.02
8	I	1401	NAG	C4-C3-C2	-2.87	106.82	111.02
8	J	802	NAG	C4-C3-C2	-2.68	107.09	111.02
8	B	802	NAG	C4-C3-C2	-2.66	107.11	111.02
8	F	802	NAG	C4-C3-C2	-2.66	107.11	111.02
8	J	817	NAG	C4-C3-C2	-2.44	107.45	111.02
8	F	817	NAG	C4-C3-C2	-2.43	107.45	111.02
8	B	817	NAG	C4-C3-C2	-2.43	107.45	111.02
8	F	807	NAG	C4-C3-C2	-2.22	107.77	111.02
8	B	807	NAG	C4-C3-C2	-2.22	107.77	111.02
8	J	807	NAG	C4-C3-C2	-2.21	107.77	111.02
8	F	801	NAG	C4-C3-C2	-2.01	108.06	111.02

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	802	NAG	O5-C5-C6-O6
8	J	802	NAG	O5-C5-C6-O6
8	F	802	NAG	O5-C5-C6-O6
8	B	817	NAG	O5-C5-C6-O6
8	J	817	NAG	O5-C5-C6-O6
8	F	817	NAG	O5-C5-C6-O6
8	B	807	NAG	O5-C5-C6-O6
8	J	807	NAG	O5-C5-C6-O6
8	F	807	NAG	O5-C5-C6-O6
8	A	1401	NAG	O5-C5-C6-O6
8	E	1401	NAG	O5-C5-C6-O6
8	I	1401	NAG	O5-C5-C6-O6
8	B	801	NAG	O5-C5-C6-O6
8	B	803	NAG	O5-C5-C6-O6
8	J	801	NAG	O5-C5-C6-O6
8	J	803	NAG	O5-C5-C6-O6
8	F	801	NAG	O5-C5-C6-O6
8	F	803	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

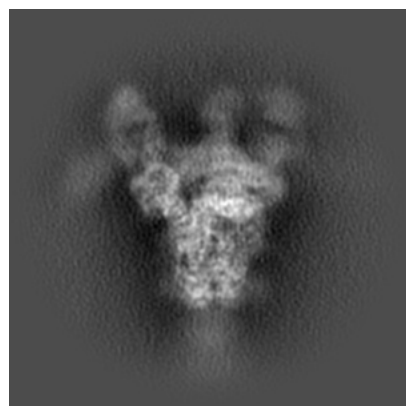
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20527. These allow visual inspection of the internal detail of the map and identification of artifacts.

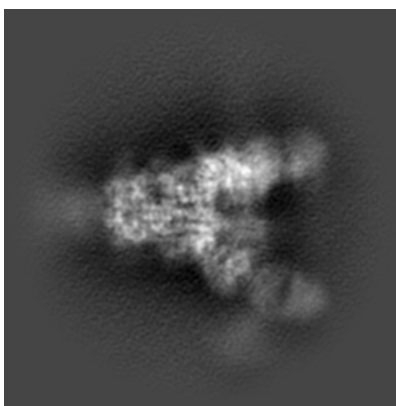
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

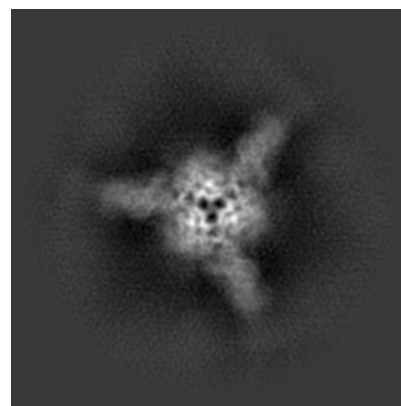
6.1.1 Primary map



X

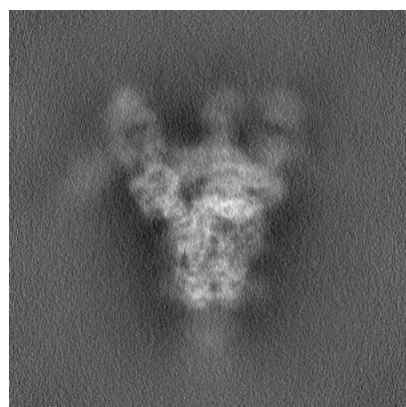


Y

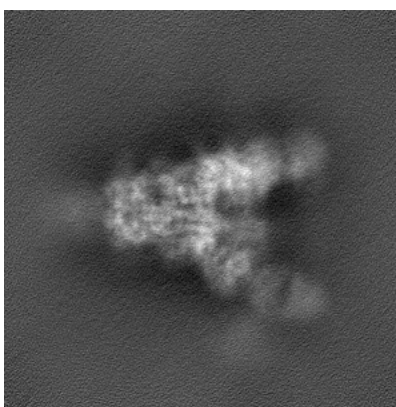


Z

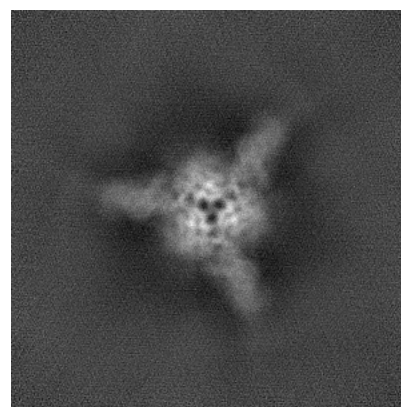
6.1.2 Raw map



X



Y

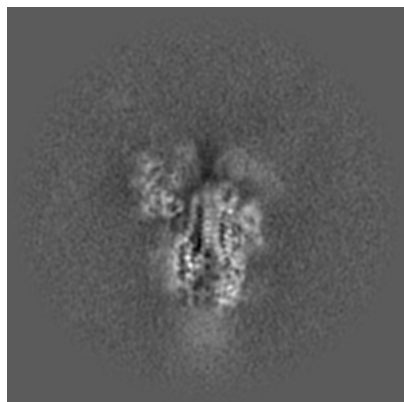


Z

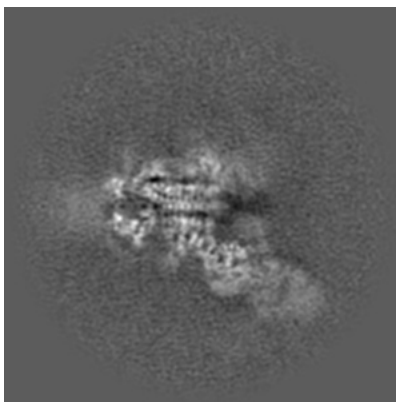
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

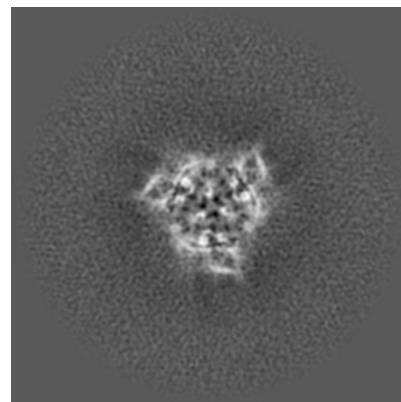
6.2.1 Primary map



X Index: 175

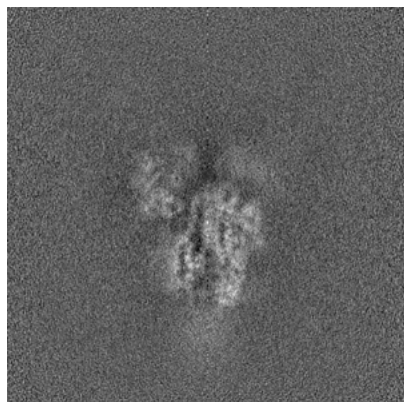


Y Index: 175

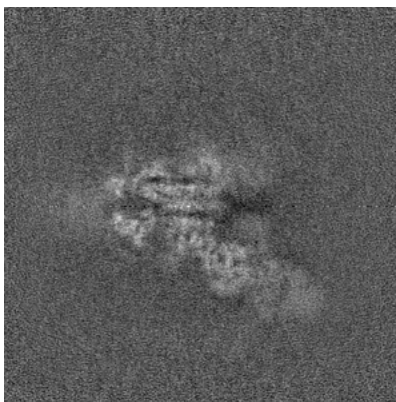


Z Index: 175

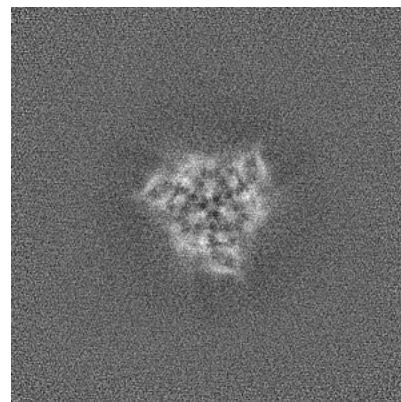
6.2.2 Raw map



X Index: 175



Y Index: 175

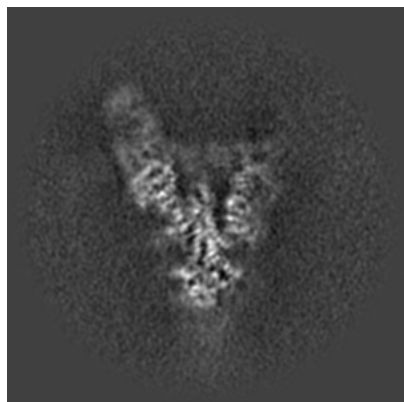


Z Index: 175

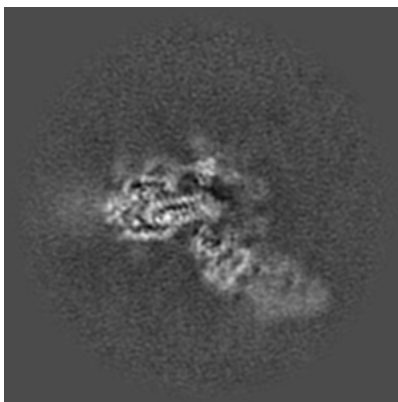
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

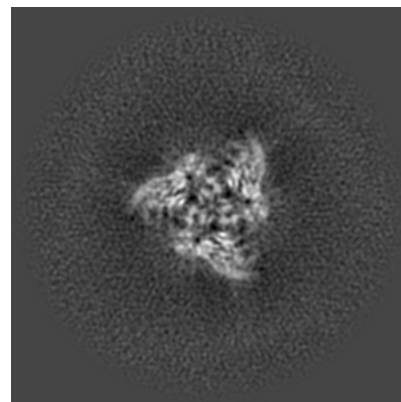
6.3.1 Primary map



X Index: 192

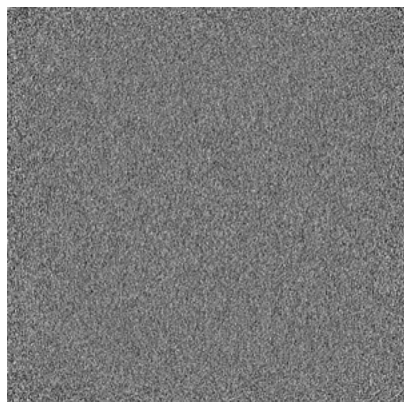


Y Index: 187

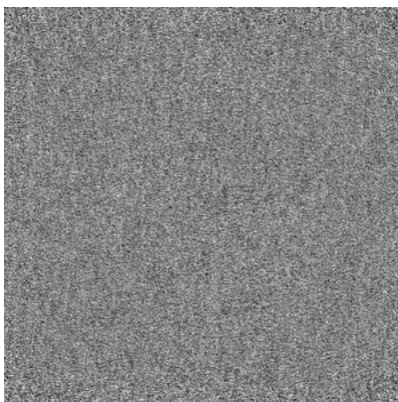


Z Index: 180

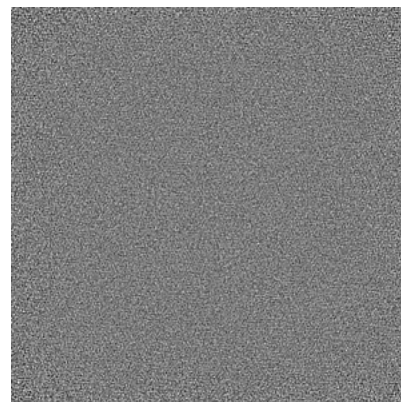
6.3.2 Raw map



X Index: 0



Y Index: 0

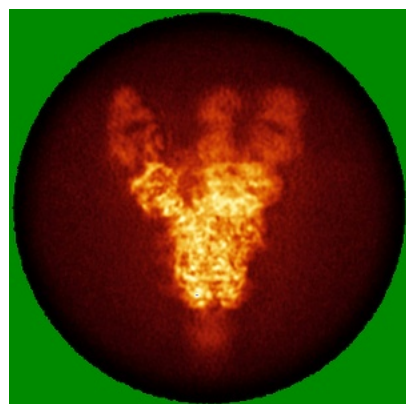


Z Index: 0

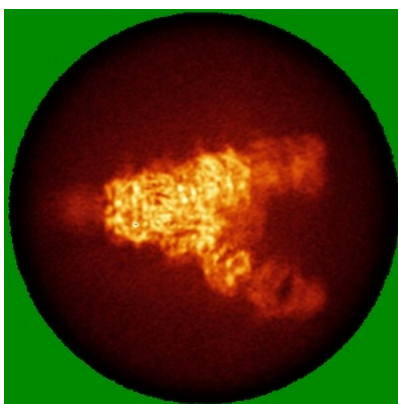
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

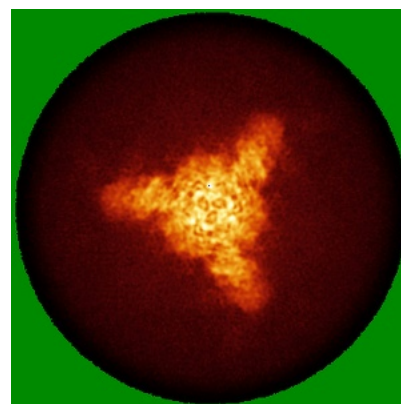
6.4.1 Primary map



X

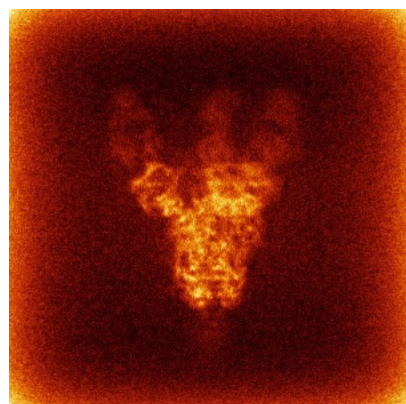


Y

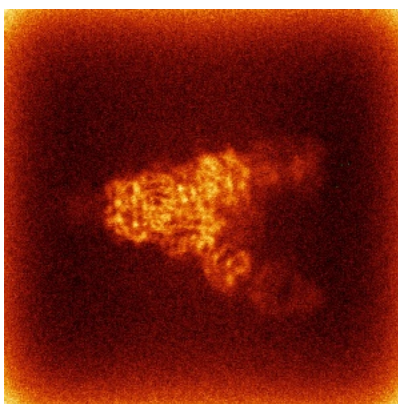


Z

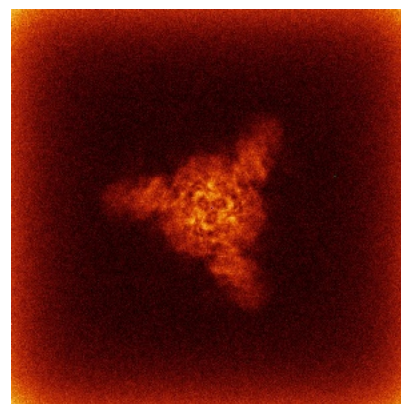
6.4.2 Raw map



X



Y

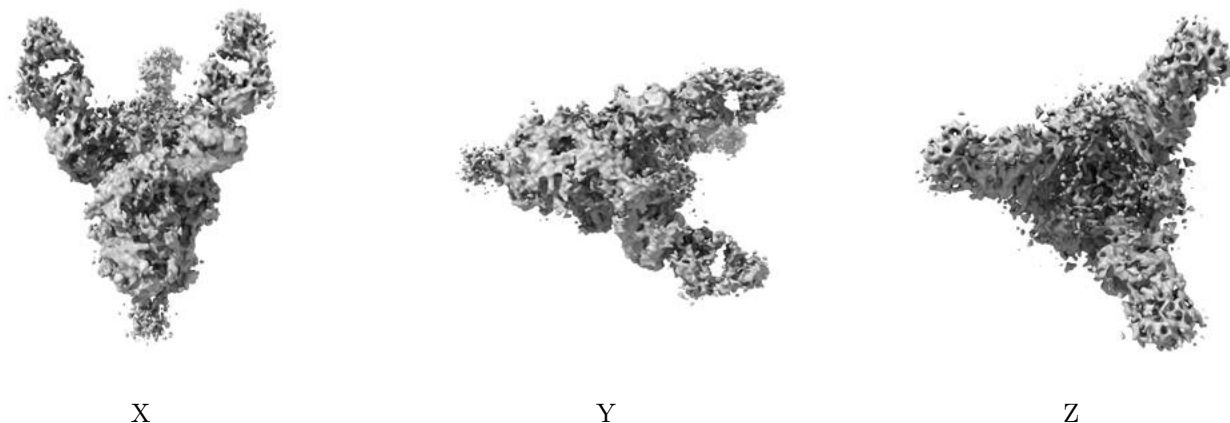


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

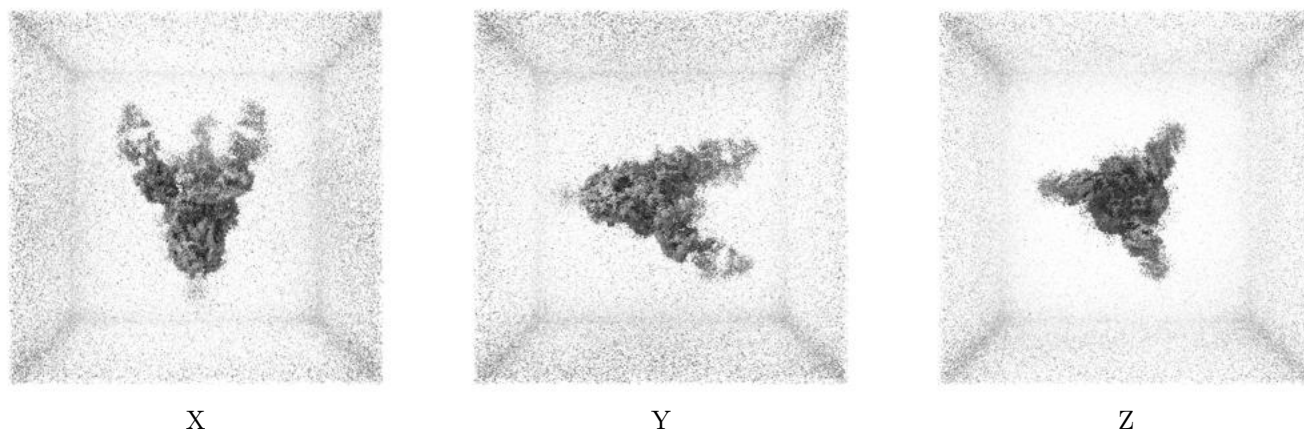
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.264. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

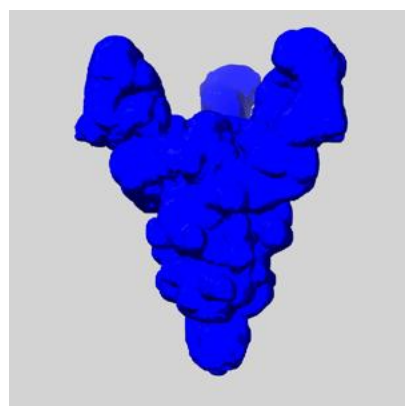
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

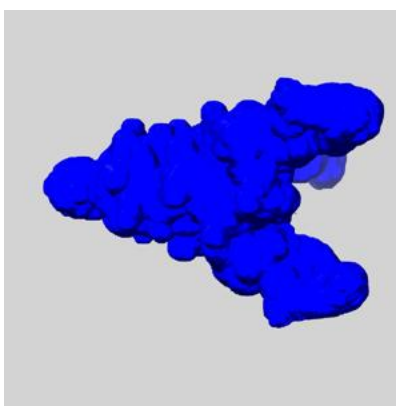
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

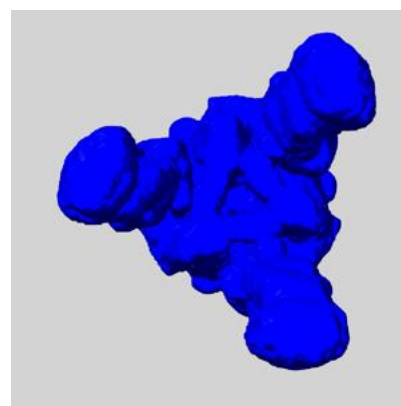
6.6.1 emd_20527_msk_1.map [i](#)



X



Y

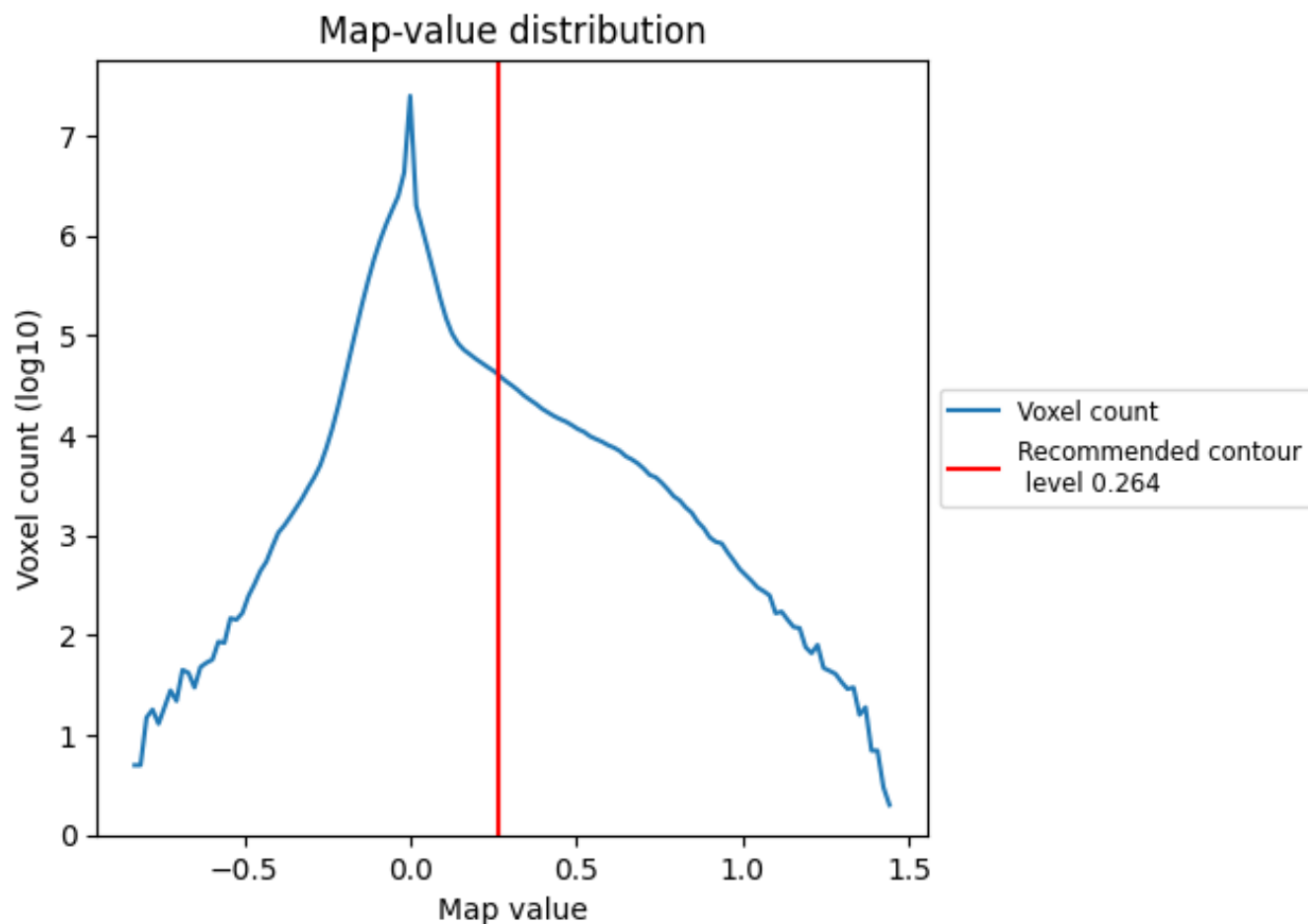


Z

7 Map analysis [i](#)

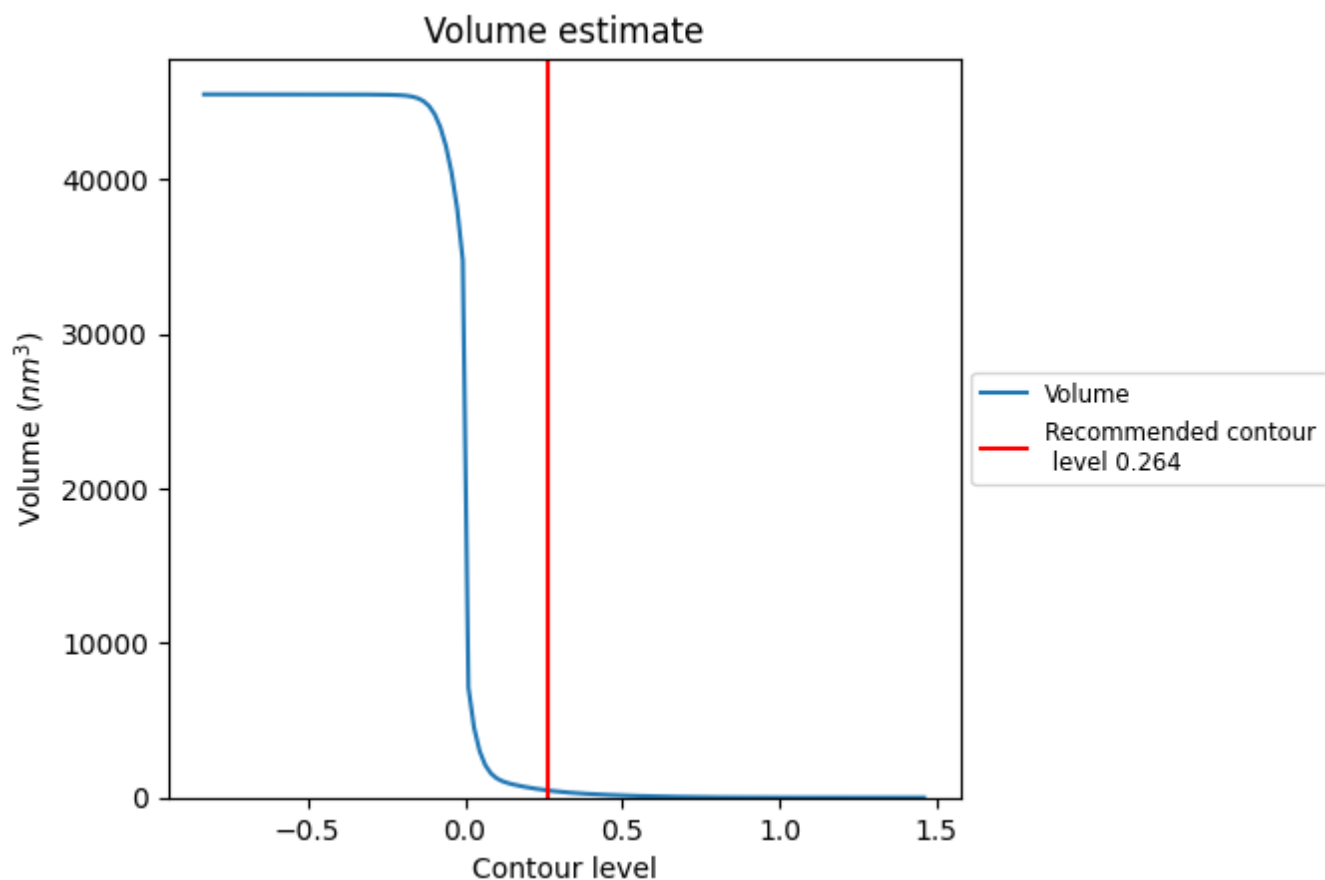
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

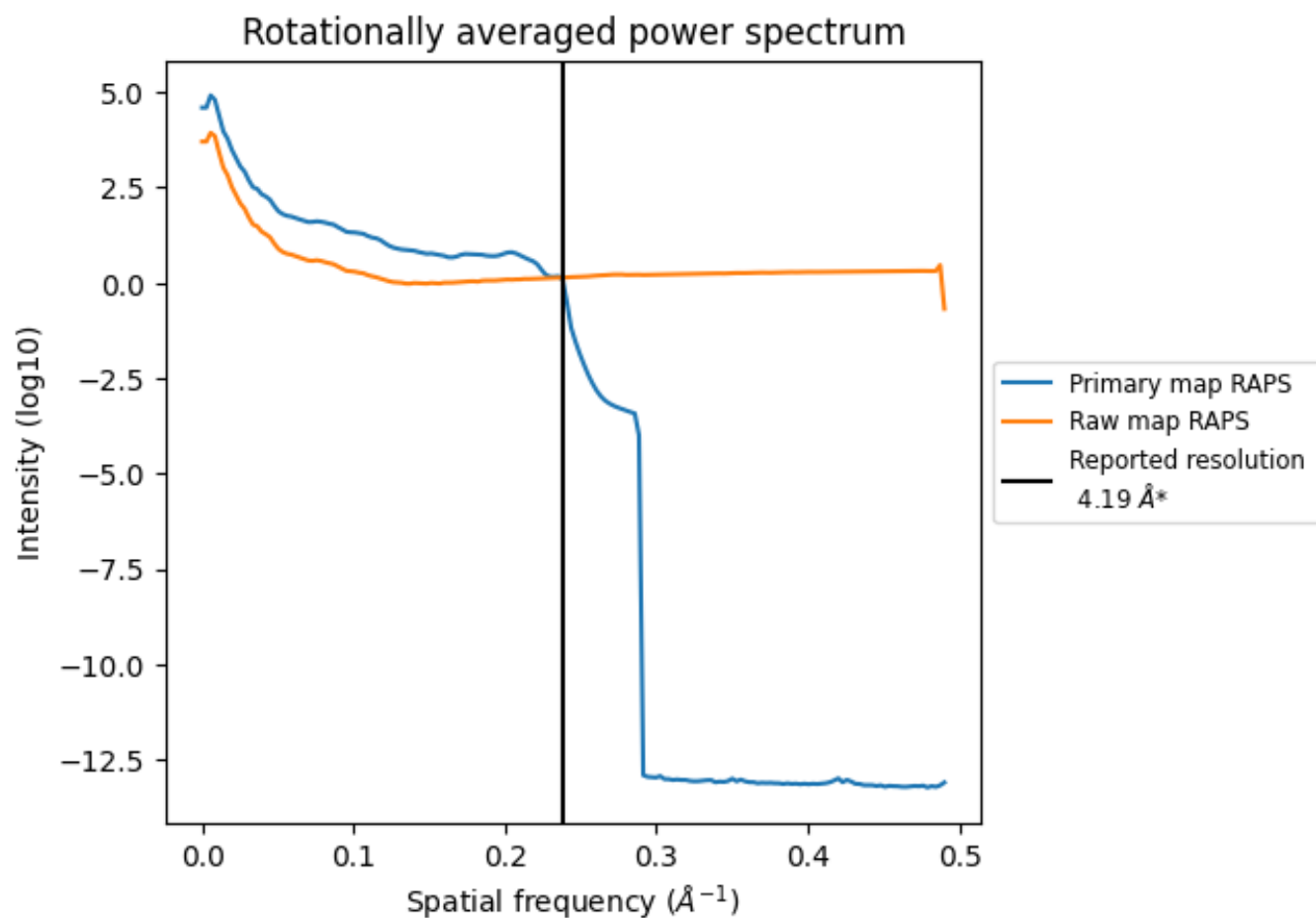
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 462 nm³; this corresponds to an approximate mass of 417 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

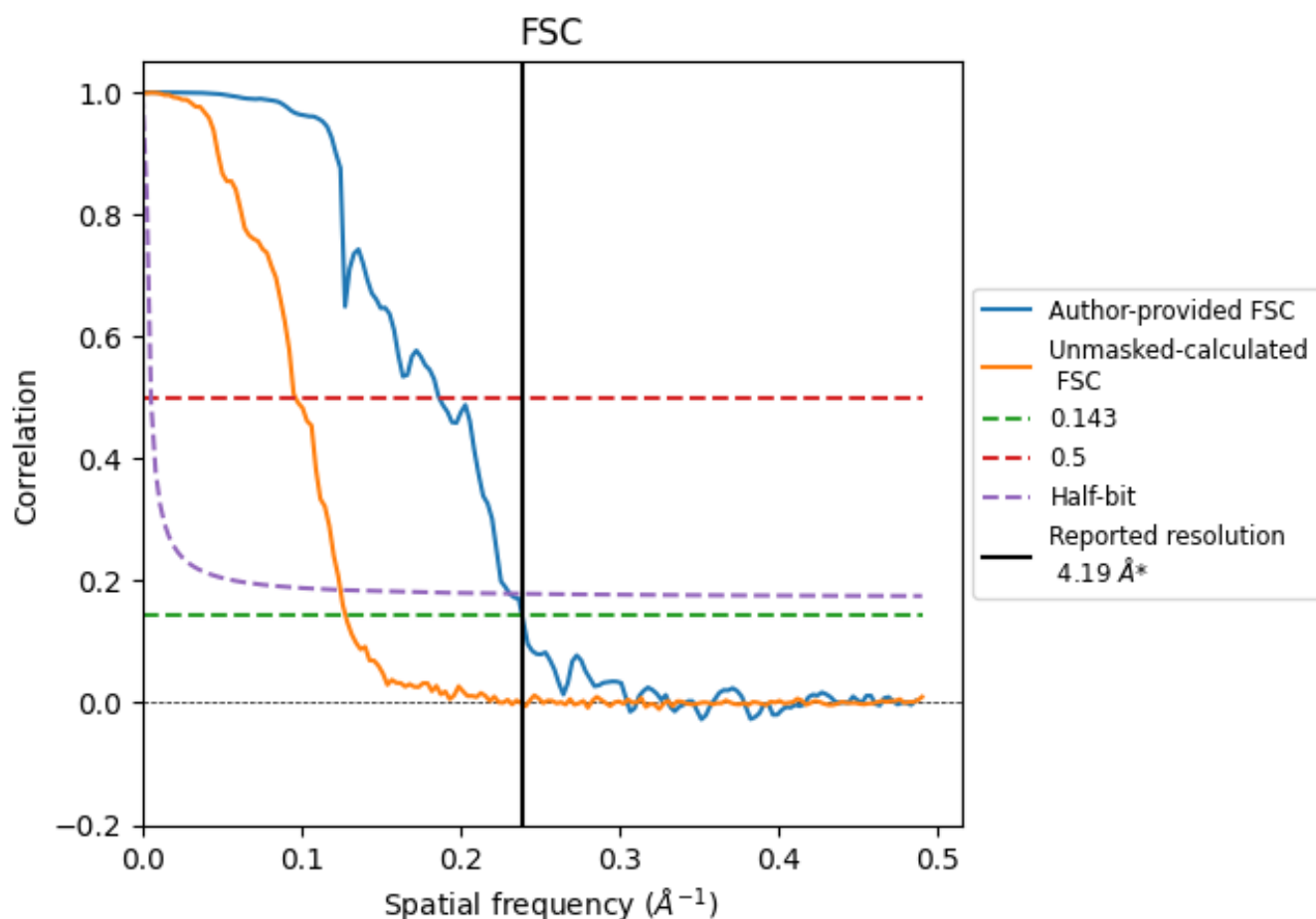


*Reported resolution corresponds to spatial frequency of 0.239 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.239 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

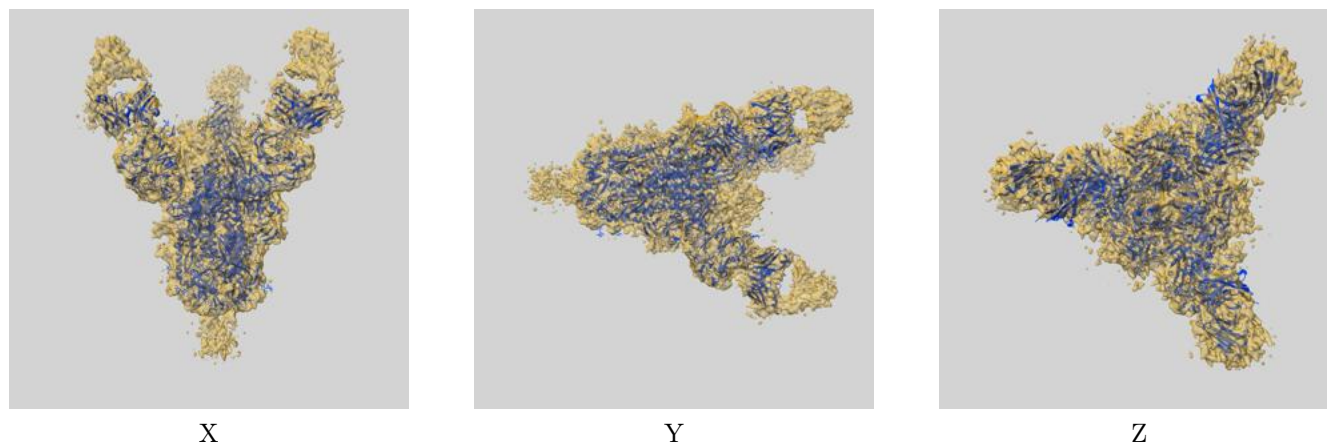
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.19	-	-
Author-provided FSC curve	4.19	5.36	4.33
Unmasked-calculated*	7.82	10.37	8.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.82 differs from the reported value 4.19 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20527 and PDB model 6PZ8. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



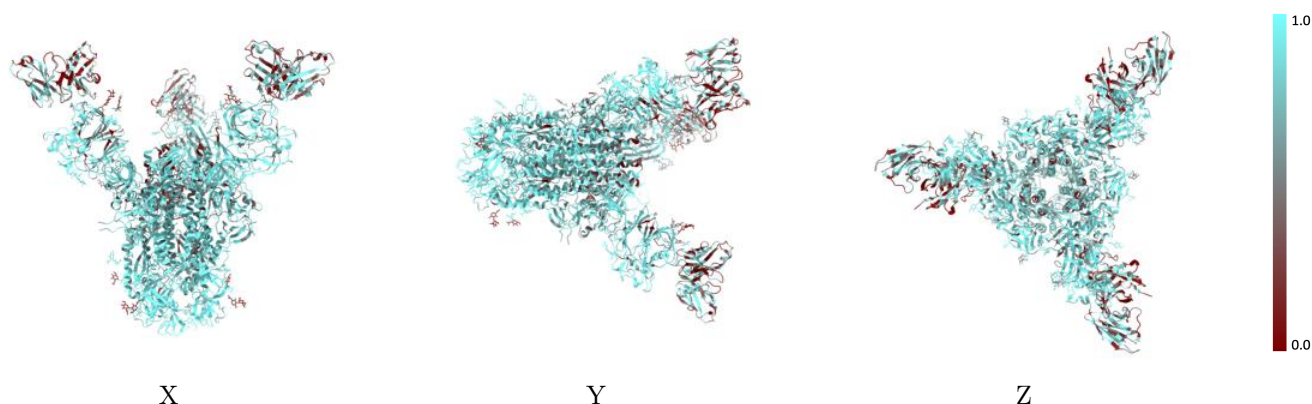
The images above show the 3D surface view of the map at the recommended contour level 0.264 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



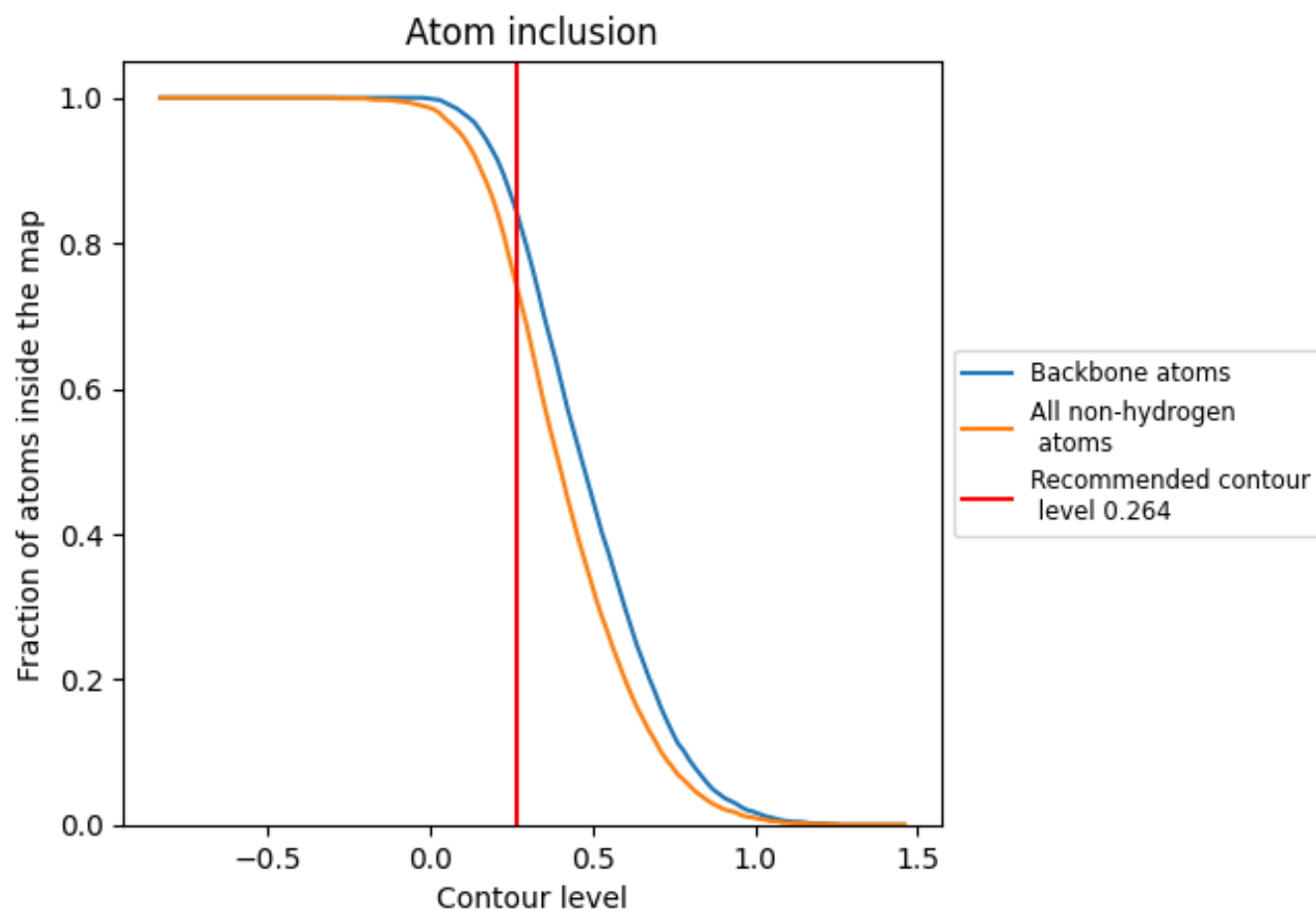
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.264).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.264) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7450	 0.1330
A	 0.8020	 0.1720
B	 0.8180	 0.1170
C	 0.4220	 0.0970
D	 0.4270	 0.0990
E	 0.8030	 0.1700
F	 0.8180	 0.1160
G	 0.5270	 0.0670
H	 0.4260	 0.0930
I	 0.8030	 0.1720
J	 0.8170	 0.1180
K	 0.5180	 0.0680
L	 0.5180	 0.0680
M	 0.5710	 0.2370
N	 0.0360	 0.1680
O	 0.8930	 0.3310
P	 0.9290	 0.2790
Q	 0.9230	 0.2700
R	 0.3930	 0.2060
S	 0.6890	 0.0050
T	 0.0000	 0.1110
U	 0.5710	 0.2540
V	 0.0360	 0.1770
W	 0.8930	 0.3340
X	 0.9290	 0.2600
Y	 0.9230	 0.2770
Z	 0.3930	 0.1960
a	 0.6890	 0.0020
b	 0.0000	 0.0970
c	 0.5710	 0.2400
d	 0.0360	 0.1530
e	 0.8930	 0.3450
f	 0.9290	 0.2600
g	 0.9230	 0.2670
h	 0.3930	 0.2150



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Chain	Atom inclusion	Q-score
i	 0.6890	 0.0130
j	 0.0000	 0.1100